The QUIC Start Guide (v 5.8)

The Quick Urban & Industrial Complex (QUIC)
Dispersion Modeling System

DRAFT

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Installation of the QUIC system

There are versions of QUIC for 32- and 64-bit Windows XP and Windows 7, 64-bit Linux, and 64-bit Intel Mac OS X. Several users have reported that QUIC also runs on Windows Vista, but it is not officially supported at this time due to LANL computer policy. Note that the 64-bit versions allow the QUIC transport and dispersion codes to access greater than 2 GB of RAM and thus larger problems can be run.

QUIC comes in two flavors: one that runs inside of Matlab® and the other that runs standalone as an executable. In theory, both versions should run identically. The Matlab version, known as the P-code version of QUIC, has the advantage of being easy to install (see instructions below), but it does require a Matlab software license. Note that Matlab 7.9 or later should be used to guarantee that the GUI functions properly. In addition, note that several routines require Matlab's Mapping Toolbox and Image Processing Toolbox.

The standalone executable version allows the user to run QUIC without a Matlab license and without purchasing extra toolboxes. Another advantage of the standalone version is that it requires less computer memory since Matlab does not need to be run simultaneously. The disadvantage is that the installation is more complicated (see instructions next page) and one needs to download a large (but free) Matlab library file.

More information about the Matlab software can be found at:

<div align="center">

http://www.mathworks.com

</div>

QUIC is available for non-profit research purposes. Contact either Michael Brown (mbrown@lanl.gov) or Matt Nelson (nelsonm@lanl.gov) to find out if you are eligible to obtain the code.

Installation instructions:

1) In your web browser, navigate to the QUIC web site at

<div align="center">

http://www.lanl.gov/projects/quic/index.html

</div>

2) Click on the "downloads" tab and enter your user name and site password.

P-Code version of QUIC

3) Follow the instructions on the web page and download the *QUIC_pcode.zip* file to your computer.

4) Using the zip file password, unzip the *QUIC_pcode.zip* file into any directory on your computer.   You are now ready to run QUIC!

Standalone Executable Version of QUIC

For the executable version of QUIC, you need to download two items: the Matlab Component Runtime (MCR) installer file and the QUIC archive package. The former contains Matlab libraries that are required for the graphical user interface to function properly.

3) From the link on the QUIC web page, download the latest Matlab Component Runtime (MCR) installer file for the Windows, Linux, or Mac OS X platform.

4) Unzip the MCR installer file for your system.
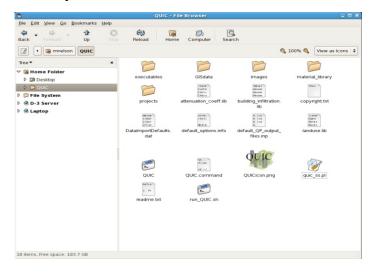
32- and 64-bit Windows
5) Double click on the MCR installer file and follow the instructions of the install wizard.

6) Create a QUIC folder in the desired location and extract the contents of the QUIC archive package into it.

64-bit Linux
5) After downloading the MCR installer file for Linux, change the permissions of the file to make it executable.

6) As root, run the MCR installer file from a terminal and follow the instructions of the installation wizard. Use the default install location if you wish to use the simplified launching procedure described immediately below.

In order to use the simplified installation of QUIC on Linux you will need to follow these instructions:

i. Create a directory named "QUIC" in your home directory.

ii. Extract the contents of the QUIC archive package into the QUIC directory. The contents of the directory should now be as shown below:

iii. Now drag the QUIC.command file onto your Panel. This will launch the Create Launcher window.

a.

iv. Enter the name of the launcher link (i.e., QUIC) and click on the "No Icon" button and then the "Browse" button in the Browse Icons window to navigate to the QUICicon.png file included in the archive package.

a.

v. Select the QUICicon.png file and press "OK" in both the Browse Icons and the Create Launcher windows. This will create a launcher icon in your panel as seen below:

vi. To launch QUIC simply click on the icon on your panel. All of the environment variables are automatically set at launch time by the shell scripts.

64-bit Intel Mac

5. Change the permissions of the MCR installer file to make it executable.

6. Double click on the MCRinstaller_MACI.dmg file and follow the instructions of the installation wizard. Use the default install location if you wish to use the simplified launching procedure described immediately below.

In order to use the simplified installation of QUIC on Mac OS X you will need to follow these instructions:

   i.   Create a directory named "QUIC" in your Applications directory.

   ii. Extract the contents of the QUIC archive package into the QUIC directory. The contents of the directory should now be as shown below:

   a.

   iii. Now drag the QUIC.command file onto your dock. This will create a launcher icon in your dock as seen below:
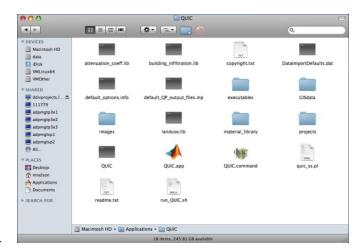

   a.
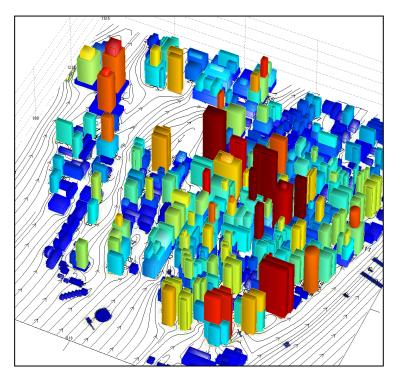
   iv. To launch QUIC simply click on the icon on your dock. All of the environment variables are automatically set at launch time by the shell scripts.

What is QUIC?

QUIC stands for the Quick Urban & Industrial Complex (QUIC) dispersion modeling system. QUIC is a fast response urban dispersion model that runs on a laptop. QUIC is comprised of a 3D wind field model called QUIC-URB, a transport and dispersion model called QUIC-PLUME, and graphical user interface called QUIC-GUI. QUIC also includes QUIC-PRESSURE to solve for pressure fields in and around buildings, a population exposure assessment tool called QUIC-POP, and an indoor infiltration calculator for computing indoor concentrations. Transport and dispersion for different types of airborne contaminants can be computed on building to neighborhood scales in tens of seconds to tens of minutes. QUIC will never give perfect answers, but it will account for the effects of buildings in an approximate way and provide more realism than non-building aware dispersion models.

QUIC-URB
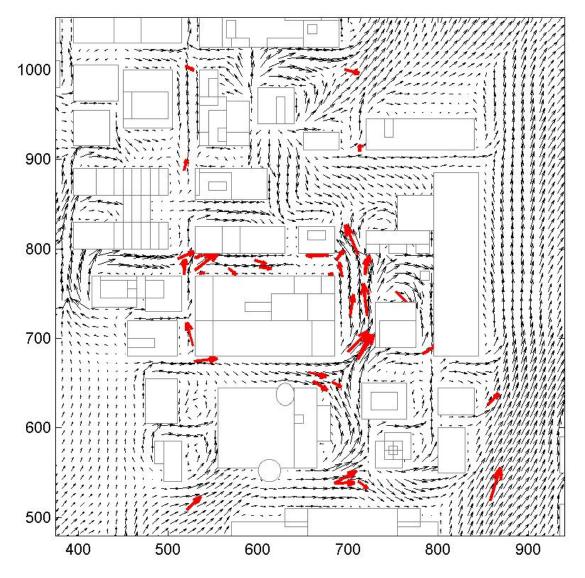
QUIC-URB is a fast response model for computing flow fields around buildings. It uses empirical algorithms and mass conservation to quickly compute 3D flow fields around building complexes. The underlying code is based on the work of Röckle (1990). Improvements to the original model are described in Bagal et al. (2003), Pol et al. (2006), Nelson et al. (2008), and Nelson et al. (2009), and Brown et al. (2009). Evaluation studies of QUIC-URB have been performed by Pardyjak & Brown (2002), Bowker et al. (2004), Clark and Klein (2006), Singh et al. (2008), and Neophytou et al. (2010). Below is an example QUIC-URB output showing streamlines near street level in Lower Manhattan.

Streamlines in the X-Y plane showing how the air near street
level flows around buildings in Lower Manhattan.

QUIC-CFD
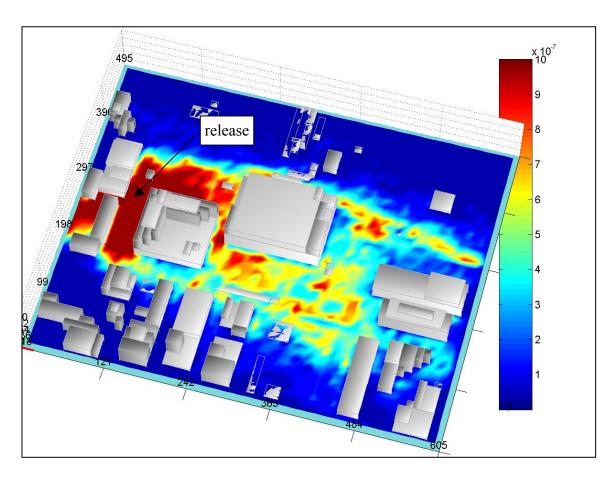
A simple computational fluid dynamics code called QUIC-CFD has been added to QUIC as a wind solver option. Although it is significantly slower than QUIC-URB, it should yield more realistic wind field solutions. In order to make the QUIC-CFD code faster than traditional CFD codes, Gowardhan et al. (2010) used a simple one-equation turbulence model with a diagnostic turbulent length scale and the name of solution scheme (based on Chorin). The code has been evaluated by Gowardhan et al. (2010) and Neophytou et al. (2010). An example of the wind field produced by the model is shown below.

Predicted (in black) and measured (in red) 30-minute-averaged near-surface winds in central downtown Oklahoma City (Joint Urban 2003 Field Experiment, IOP2).

QUIC-PLUME
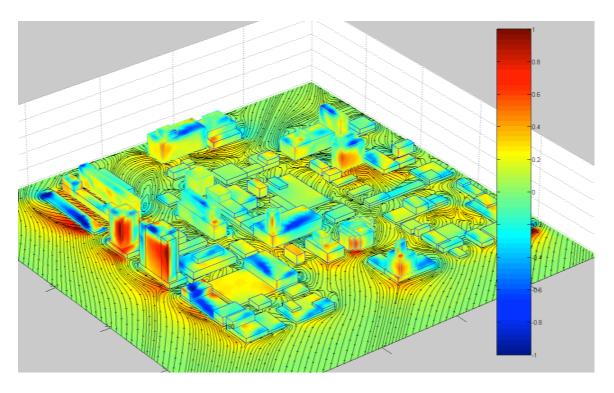
QUIC-PLUME is a Lagrangian random-walk dispersion model for computing concentration and deposition fields around buildings. It has been adapted to work in the inhomogeneous environment of cities. It includes reflection terms for building and street surfaces and has more terms than the normal random-walk model in order to account for the 3D gradients in turbulent and mean flow fields. The dispersion of aerosols and gases can be simulated, including deposition, gravitational settling and decay. Buoyant rise for explosive releases and dense gas heavier-than-air releases are also treated. Algorithms have been developed to account for droplet evaporation and gas-droplet two-phase plumes. The code has been tested for both idealized and real-world cases (e.g., Zajic et al., 2010; Brown et al., 2009; Allwine et al., 2008; Gowardhan et al., 2006; Williams et al., 2004). See Williams et al. (2004) for more information on the specifics of the code.

Example output from the QUIC-PLUME model showing
a contour plot of concentrations in the X-Y plane for a region in Boston.

QUIC-PRESSURE
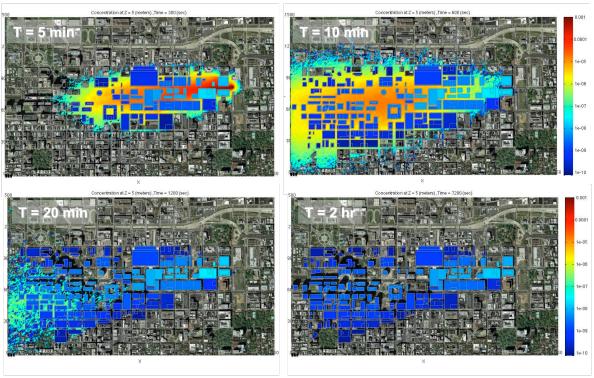
Using the mean 3D velocity field produced by QUIC-URB, QUIC-PRESSURE solves for the 3D pressure fields through use of the pressure Poisson equation. Since only mean velocities are used in the computations, all turbulent contributions to the pressure field are neglected. More details on the pressure solver equations and evaluation studies can be found in Gowardhan et al. (2006), Brown et al. (2007), and Gowardhan et al. (2010).

The image above shows the surface pressure coefficient for the Salt Lake City domain along with the near surface streamlines. The wind and pressure fields were created in 67 seconds and 45 seconds, respectively, using a 2.5 GHz Pentium 4 processor.

QUIC-INDOOR

QUIC-INDOOR allows the user to approximate concentrations inside of buildings from an outdoor release. The methodology is based on Hall et al. (2000) and has been modified by Werley (2007) to account for filtration systems, indoor deposition, agent decay, air recirculation, and exfiltration. The approach is very simplified in that buildings are treated as well-mixed volumes and infiltration and air intake locations are not based on real building information, but rather an array of points on each building face spaced at the grid cell resolution. QUIC-INDOOR comes with a default list of building types (e.g., leaky or air tight residential, old office with open or closed windows, modern office with HEPA filter) that contain different leakiness and filtration efficiency parameters based on Chan et al. (2003), Chan et al. (2004) and Persily and Gorfain (2004). Since QUIC can track particles of different sizes, the filtration scheme accounts for size-dependent filtration efficiencies and size dependent deposition. QUIC-INDOOR is a sub-routine inside of the QUIC-PLUME model.
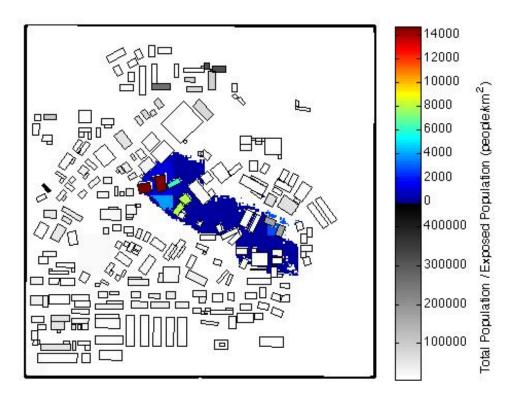

Outdoor and indoor concentrations at 5, 10, 20, and 120 minutes after the outdoor release. After 20 minutes the plume has nearly traveled out of the downtown area, but indoor concentrations remain long after the plume has gone.

QUIC-POP

QUIC-POP utilizes the 2005 LANL Day-Night Population Database (McPherson and Brown, 2003; McPherson et al., 2006) to compute population exposures. The database comes packaged with QUIC in the *GISdata* folder inside of the QUIC *code* folder. The population database contains population numbers for the entire continental US at roughly 250 m resolution. The nighttime population is a slightly modified version of the US Census Bureau database and represents residential population. The daytime database includes the worker and daytime residential population. Note that there are numerous limitations to the database, including no school, in-transit, special event, or tourist populations (see McPherson et al. (2006) for further details).

After computing the plume transport and dispersion, QUIC-POP allows for relatively easy calculation of the number of people exposed to different user-specified thresholds of concentration, dosage, or deposition flux. In addition, QUIC-POP contains a volume-based algorithm for attributing people to buildings, allowing for estimates of indoor population exposures. The image below shows an example of population exposed due to an accidental release of ammonia.

A chemical release resulted in a subset of the population in the domain being exposed above a threshold value (colored regions). In this example, exposed population in persons per km^2 was computed for both outdoor population and indoor population.

QUIC-GUI

The QUIC-GUI is the graphical user interface that allows one to set-up problems, run the wind and dispersion codes, and visualize results. The rest of this document describes how to use the QUIC-GUI.

Starting the QUIC-GUI
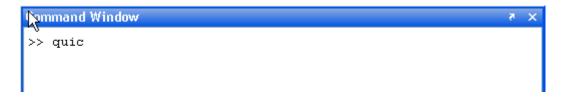
P-Code Version

a) Launch Matlab®

Make the Matlab working directory the folder containing the QUIC files. Set the Current Directory to the folder named "*code*" or "*pcode*".

directory containing QUIC files

b) On the Matlab® Command Line type "quic".

c) The QUIC-GUI Main Window will now show up (as shown below on the next page.

Standalone Executable Version

a) On Windows systems

  i) Navigate to *<QUICroot>\code*
  ii) Double click on the *QUIC.exe* file to bring up the QUIC-GUI Main Window.

b) On Mac OS X and Linux systems

  i)   Open a command terminal
  ii) Navigate to *<QUICroot>/code*
  iii) Type "*quic.exe*" to bring up the QUIC-GUI Main Window.

The QUIC-GUI Main window will open. This screen contains, from left to right, buttons for creating, opening and saving projects, specifying the input parameters for the QUIC-URB wind model (building layout and meteorological inflow), running QUIC-URB, specifying the input parameters for the QUIC-PLUME dispersion model (source term specification, concentration grid setup, and random-walk parameters), running QUIC-PLUME, visualizing the model output, exporting data, computing pressure fields, and estimating population exposure.
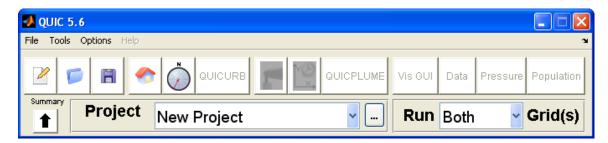
The sequence of steps in setting up and running the QUIC models proceeds from left to right (City Builder > Met Builder > QUIC-URB > Source Term > Grid Setup > QUIC-Plume). Buttons are grayed-out (deactivated) until the prior steps are completed. The Vis-GUI becomes activated once output is produced by the QUIC-URB wind model.
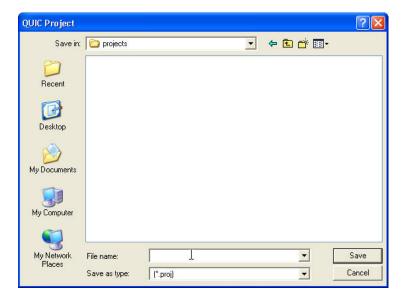
Now a new project needs to be created or an existing project needs to be opened.
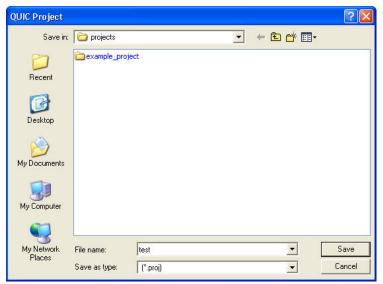
Creating a new project

A new project can be created in one of two ways when first starting the QUIC software: the first is to click the "Save" ![save icon] button immediately after start up, while the second is to proceed directly to the City Builder ![city builder icon] and the user will be prompted to save the project upon exiting from the City Builder.

- In either case, a pop-up window will open:

- In the pop-up window select the folder into which you want to save your project. A convenient choice is the *QUICroot/projects* directory. However, project files can be saved in any folder on your computer. Below is an example folder structure:
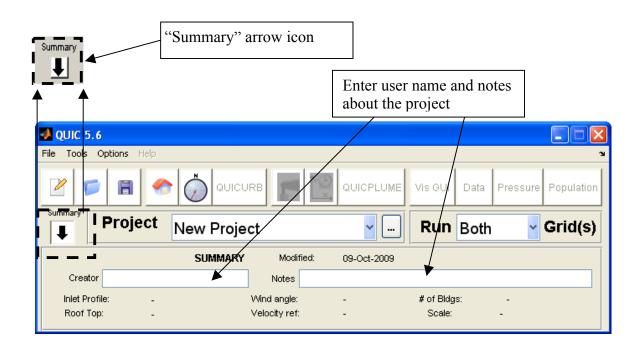
- Type in the file name (note: this name will also be used to name your project folder). Then press 'Save'. A project folder will be created which contains project files (*.*proj*) and the nested grid project subfolders.

- The last directory where a project was saved is written into the *default_options.info* file located in the *pcode* folder and the GUI will use this location as the default projects folder the next time that it is opened.

If the user is already working on a project and wants to start a new project, the "New Project" ✎ button can be clicked and the existing project will be removed from GUI memory and all values will be set to their default value (note that you can lose the existing project, if you have not previously saved the project).

Optional Step:

Press the "Summary" arrow icon on the Main-GUI to reveal the hidden project information panel (see below). Here one can enter the name of the creator of the project and notes about the project. Other information about the project parameters will also show up as soon as these values are entered in other set-up GUI's.

"Summary" arrow icon

Enter user name and notes about the project
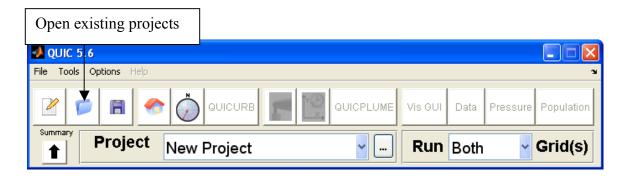
Opening existing projects
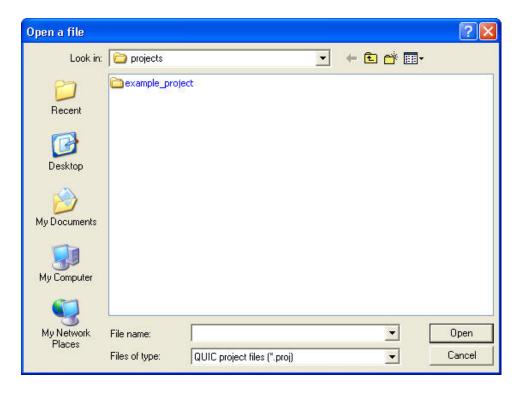
There are two options for opening existing projects: the first using the "Open Project" button and the second using the "Project Name" pull-down menu .

Open Project
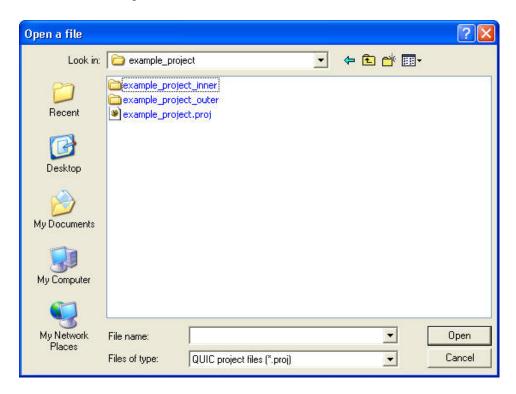
To open an existing project press the "Open Project" button :

Pressing the "Open" button opens a browse window.   Navigate to the *QUIC/root/projects* folder or wherever you have saved the QUIC project of interest.
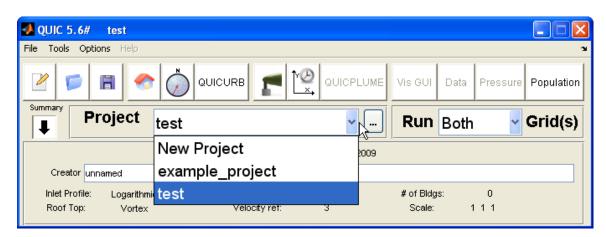
Double-click on the project folder of interest and then select the *.proj file. This project will now be loaded into QUIC-GUI. This is show below.

Project Name Pull-Down Menu

Existing projects can also be opened using the Project pull-down menu
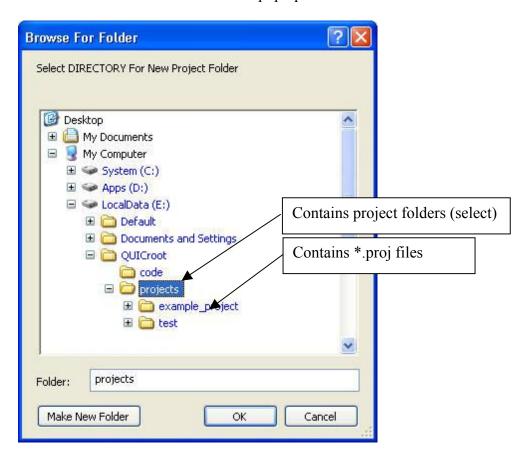
In the Project Name box the pull-down selection will now show existing projects.

Browse Icon [...]
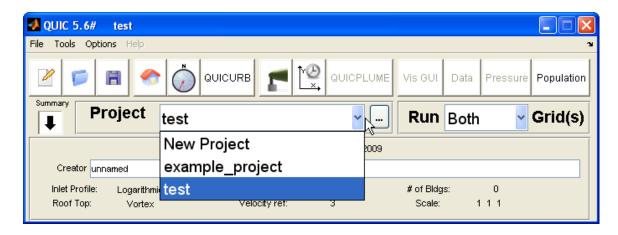
To populate the project pull-down menu with projects saved in a different project directory press the button [...].

Pressing this button launches the 'Browse For Folder' pop up window

Left-click on the project directory of interest and press the OK button at the bottom of the GUI. This will populate the Project Name Pull-Down Menu with the projects found in the new Projects directory as shown below.

The projects found in the newly selected projects directory can now be loaded from the Project Name Pull-Down Menu as was described above.

Once the appropriate project is opened, one can then proceed with setting up the parameters needed to run the QUIC-URB wind code. The first step in this process, adding or modifying buildings in the City Builder, is described in the next section.

QUIC-URB
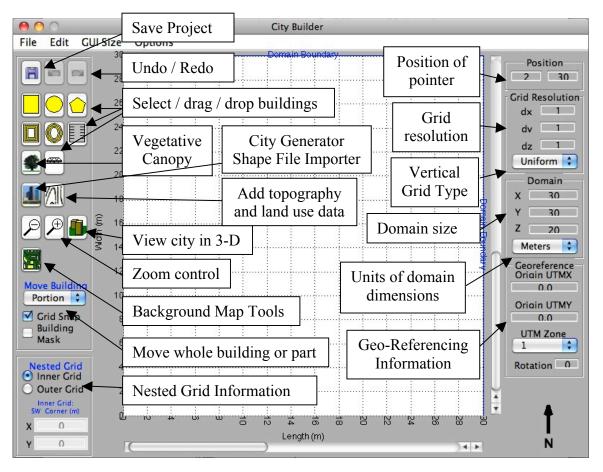
City Builder

The City Builder GUI is where the user defines the domain size, the wind field grid size, creates the cityscape composed of buildings and vegetative canopies, and can add a background map image.

- To open City Builder click on the house ![house icon] icon on the QUIC-GUI Main window:

City Builder
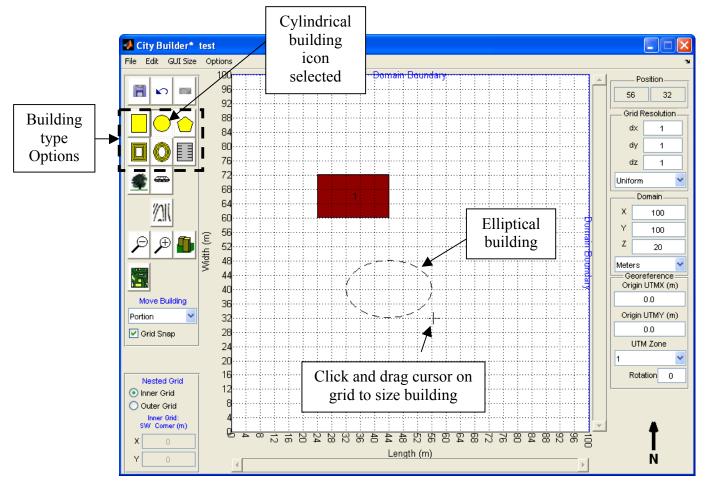
A building layout interface will open similar to the one shown below.

Add a New Building
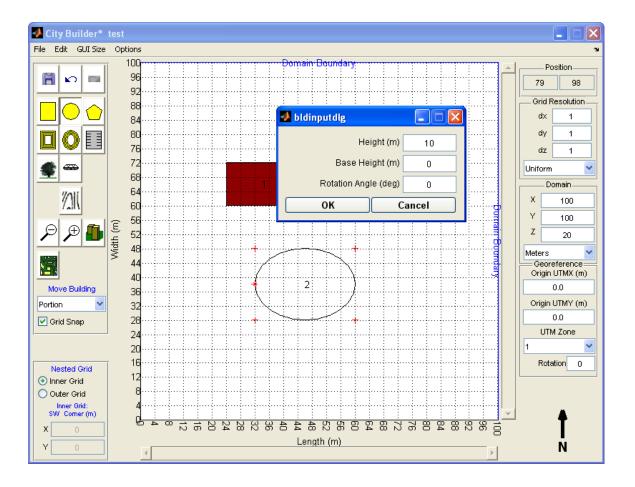
To add a new building to the project:

1) select the building type from the options on the left;

2) left-click on the grid at the location where the building is desired,

3) drag the building footprint out to the desired size and release the left mouse button.

Note: Dragging out an oblong footprint with the cylindrical building selected produces an elliptical building.

After dragging out the building footprint, a pop-up window for building height appears after dragging the building footprint:
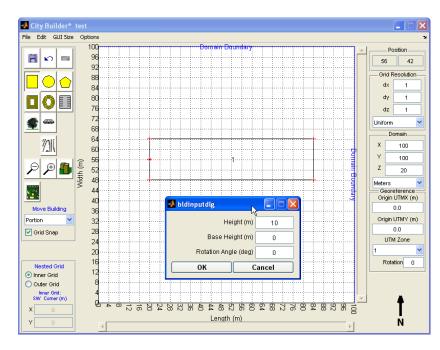
4) Enter the desired height and click OK.

There are two other inputs, the "Base Height" and the "Rotation Angle" that we ignore for now and will cover in the sections below. First we discuss the building types that are available for use in QUIC.

Obstacle Types
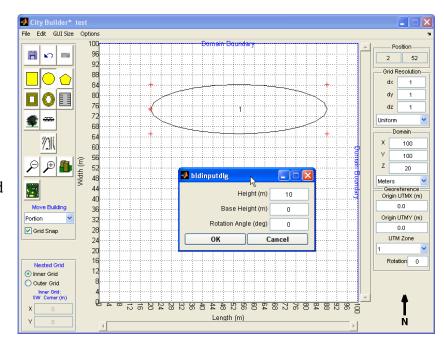
Rectangular Building

Selecting the ▢ button allows the user to add a rectangular building to the domain. The user then creates the building by simply dragging out the non-rotated footprint and then typing in the height, and if necessary, the base height and rotation angle in the pop-up window. Note that the height of the building is relative to the base height.

Elliptical Building
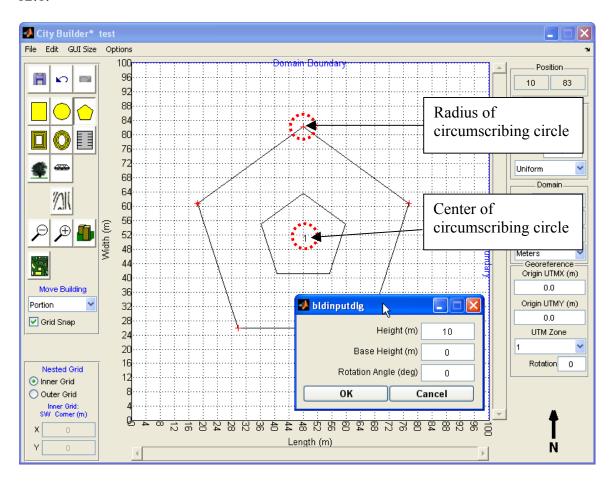
Selecting the ⬭ button allows the user to add an elliptical building to the domain. Similar to the rectangular building, the user can resize the building by dragging out the non-rotated footprint and then typing in the height, the base height and the rotation angle in the pop-up window. Note that the curved sides of the elliptical building are approximated on the orthogonal grid in a "stair step" fashion with all of the cells with centers

inside the elliptical footprint denoted as building cells.
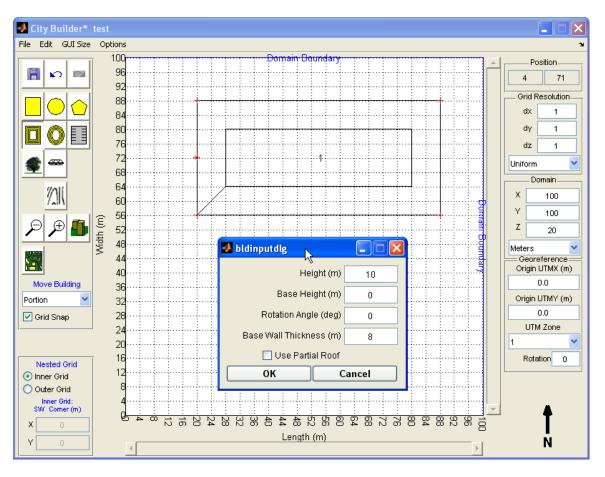
Pentagon Building

Pentagon-shaped buildings can be added to the domain by selecting the [icon] button. The method for dragging out a pentagonal building is different from that used to define rectangular and elliptical buildings. A circumscribing circle defines the pentagonal building. As such a pentagon is produced by left-clicking on the center of the circle and dragging out the radius of the circumscribing circle. The radius defining the courtyard of the pentagon building is hardwired to be 40% of the radius defining the size of the building. Due to the highly specialized nature of the pentagon-shaped building, the flow algorithms in QUIC-URB have been tuned for the 12:1 radius to height ratio characteristic of the Pentagon building. The flow fields produced from these algorithms may not be appropriate for radius to height ratios that are dramatically different from 12:1.
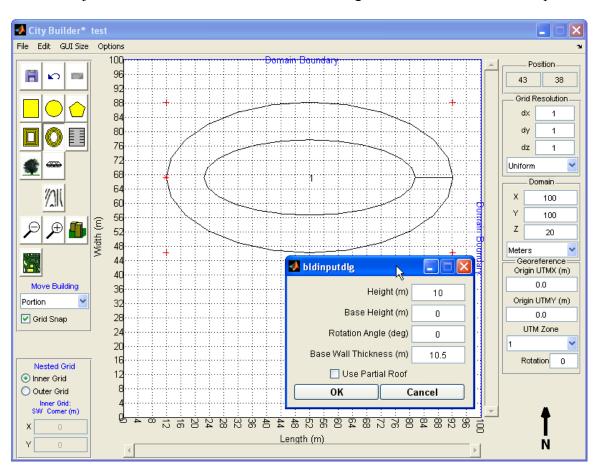
Rectangular Stadium

Open-air rectangular stadiums can be added to the domain by selecting the ▣ button. The rectangular stadium is defined in a similar way as a simple rectangular building, except that stadium "courtyard" (i.e., playing field) and roof type must be specified. The stadium courtyard is defined by a base wall thickness. The stadium walls start at this thickness at the base of the building and taper to a single grid cell thick at the top of the building. If a partial roof is selected, the lower 80% of the building height will be used for the stands and the upper 20% will be used for the roof. The opening in the roof has the same footprint as the opening in the base. The roof is visualized as being an infinitely thin shell with a parabolic cross-section with the steepest slopes near the outer edge of the building. This idealized shell is approximated as being a single grid cell thick.
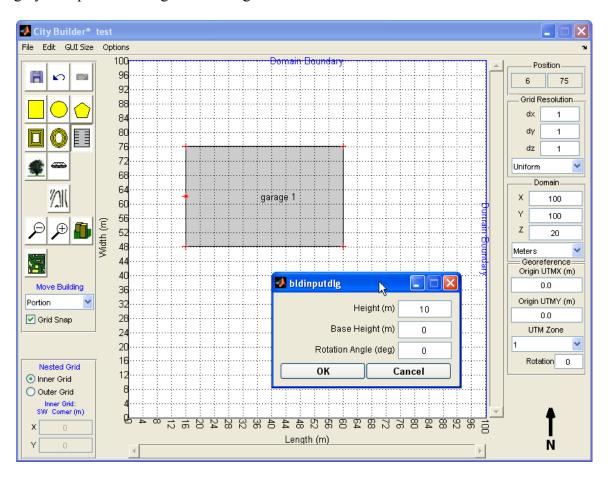
Elliptical Stadium

Elliptical stadiums can be added to the domain by selecting the ⊙ button. The elliptical stadium is defined in the same way as the rectangular stadium. The opening in the base is defined by an ellipse with major and minor axes that are the base wall thickness smaller than the major and minor axes that define the outer edge of the overall stadium footprint.

Parking Garage
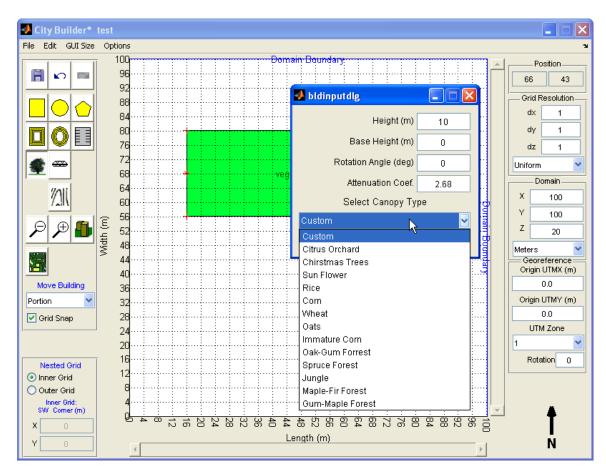
Parking garages can be added to the domain by selecting the ⊞ button. The user adds a parking garage in the exact same way as a standard rectangular building. The only difference is that a parking garage must have a height that is an even number of grid cells. This is because the parking garage is constructed of alternating horizontal layers of porous and solid grid cells. The porous layers allow the wind to pass through but slow it to 50% of its initial magnitude (Schmidlin et al., 2004). Parking garages are visualized as grey transparent rectangular buildings.

Warning: We have not been able to find detailed wind measurements around or inside of parking garages. Hence, the parking garage building shape should be used with caution.

Vegetative Canopy
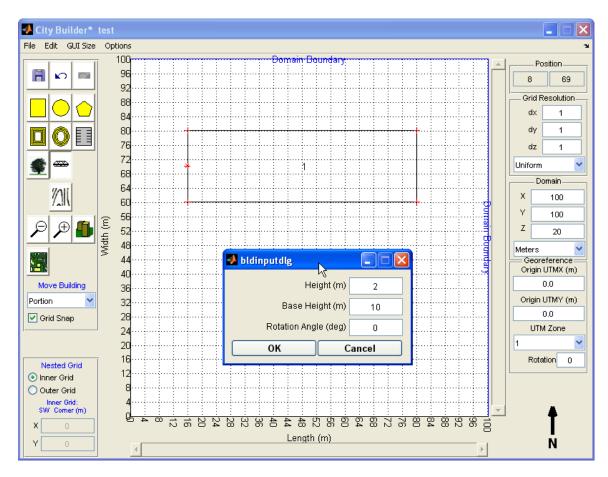
Vegetative canopies can be added to the domain by selecting the ![tree icon] button.   The vegetative canopies approximate the bulk drag effects of a forest or an agricultural field on the mean air flow. Vegetation canopies are rectangular and are defined using the same procedure as rectangular buildings. The sole difference is the additional input of the attenuation coefficient which must be defined at the same time as the height of the canopy. The attenuation coefficient determines the exponential velocity profile within the canopy (Cionco, 1965). The user can enter the attenuation coefficient manually or select one from a library of attenuation coefficients from Cionco (1978). Selecting a canopy type from the pop-up menu will populate the attenuation coefficient edit box with the value from the library. This value can then be modified to further fine tune the value for the canopy you are trying to simulate.

Note that vegetative canopies are especially useful on the outer grid, where forests cover large regions of space (and furthermore is the only type of obstacle that can be placed in the outer grid, i.e., the buildings described above can only be placed on the inner grid). One can also "trick" the QUIC model by using the vegetative canopy obstacle type to define urban regions (i.e., urban canopy) on the outer grid.

31
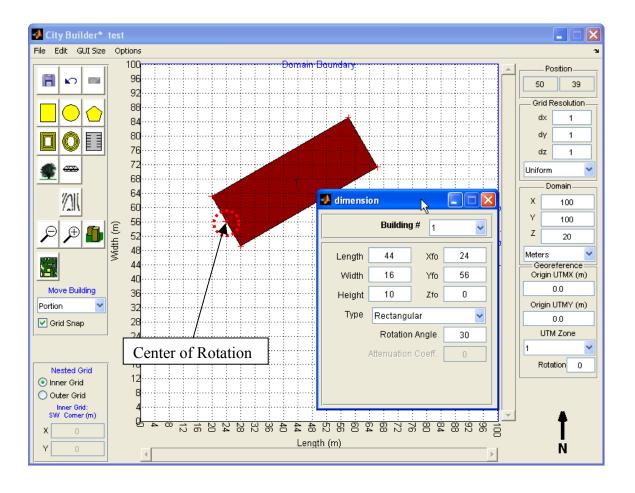
Bridge (Beta)

Bridges can be added to the domain by selecting the bridge button. The only difference between a bridge and a standard rectangular building is that the wake algorithms for the bridge obstacle assume that the obstacle is not mounted on a surface. The default values for the bridge building are different from those of a standard rectangular building: the bridge defaults to a smaller height and has a nonzero base height (recall that the height is relative to the base height).
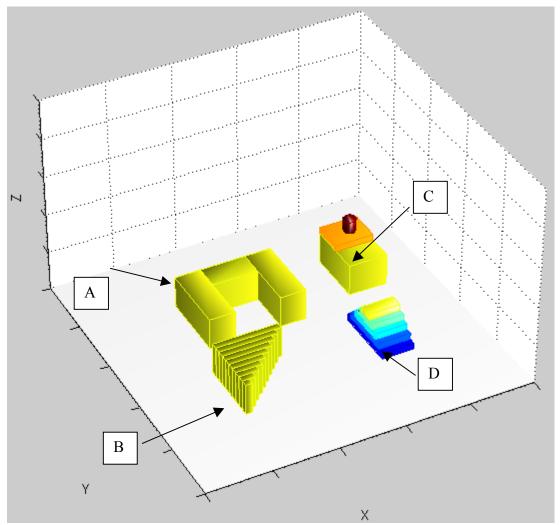
Warning: the flow algorithms for the bridge obstacle type are still under development. While the current bridge algorithms will certainly be better than using a "floating" rectangular building, the algorithms still require testing and validation against experimental data.

Obstacle Rotation

All obstacle types can be rotated relative to the orthogonal grid. The rotation angle is entered in the same Building Input Dialog pop-up window as the height (or as illustrated below can be done later in the Edit Dimensions pop-up window). Obstacles are rotated about xfo and yfo (which is the center of the pentagon building and the center of the left side for all other obstacle types). The building rotation is in degrees and a positive value will rotate the building counterclockwise. Note that the walls of a rotated obstacle will actually be stair-stepped due to the orthogonal grid that QUIC uses.

Complex buildings are made by placing multiple basic building shapes together either side-by-side and/or stacked. In this manner, L-shaped, U-shaped, and non-orthogonal (stair-stepped) buildings can be created as shown below.

Complex buildings shown above are constructed using multiple basic building shapes. The buildings shown above are colored by height. Building A has an open courtyard giving it a U-shape. Building B is an approximation of a building with a triangular footprint. Building C has a section of the roof that is higher than the rest with a cylindrical smokestack protruding from the higher portion of the roof. Building D has a pitched roof.

CAUTION! While complex building geometries can be simulated using the slice method shown in building B above, users should avoid this if possible. The building flow parameterizations were not designed for this configuration and will often produce strange results (see Nelson et al. 2008). For best results, complex buildings should be created

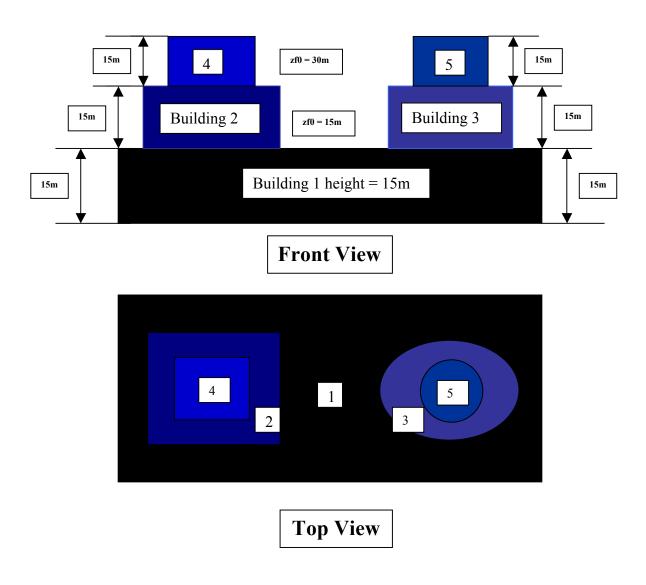using simple buildings with as large of footprints as possible. Buildings A, C, and D will all be more likely to produce realistic flow features than building B.
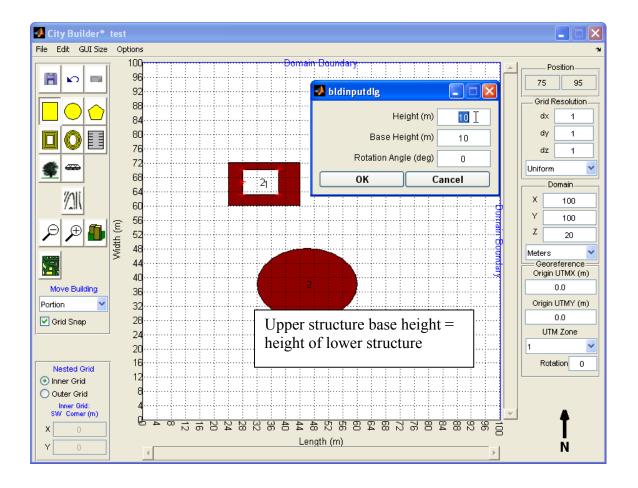
Note that the "Base Height" signifies the height at which the building base rests. A "0" implies that the building sits on the ground. A non-zero value is used when stacking the building on top of another building (see Stacking Buildings section below).

Stacking Buildings
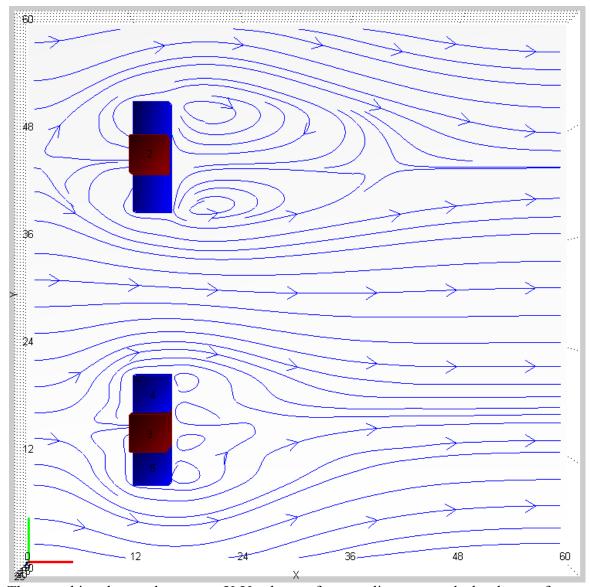
When a building is added by dragging out a shape, a pop-up window appears for setting the building height. QUIC-GUI has the ability to "stack" building shapes. 'zfo' is the base height of the building. This new parameter is needed to specify whether the building block is resting on the ground surface (zfo=0) or on another building block (zfo is then the height of the underlying building). The zfo of a new building will automatically be set to the height of the building below it if the starting point of the dragging is over another building.

In the following example the lower building (Building 1) has a height of 15 meters. Therefore, zf0 values for buildings 2 and 3 are entered as 15m. The heights of building's 2 and 3 are set to 15m. Hence, zf0 for buildings 4 and 5 are entered as 30m. Note that the height of the building is the height of the actual building block, not from the ground. So 15 m should be entered for the height of building 4, not 45 m.

Front View

Top View
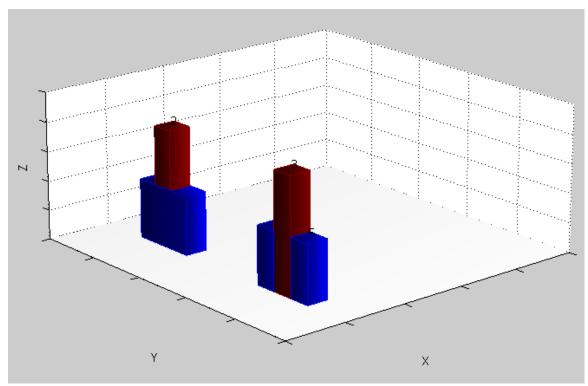
Note: Complicated building shapes may be constructed by either stacking several simple building shapes or placing them side-by-side. The QUIC-URB model has been developed to provide better results from stacked buildings. Whenever possible, buildings should be stacked, rather than placed side by side. Building structures that are geometrically identical, but built by stacking vs. side-by-side can produce different wind fields. This is shown in the figure below.

The graphic above shows an X-Y plane of streamlines around the base of two geometrically identical buildings. The building at the top of the image was created by stacking one building on top of another. The building at the bottom was created by placing three buildings side-by-side. An orthogonal view of these two buildings is found below in the View Buildings in 3D section.

View Buildings in 3D

The 3D Plot button ![icon] brings up a 3D viewer window, which allows the user to look at the buildings in 3D from different angles.

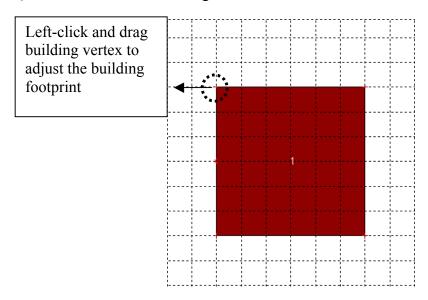This is the orthogonal view of the example above involving geometrically identical buildings that are constructed by stacking two buildings or placing three buildings side-by-side.
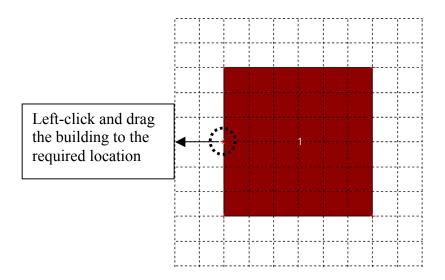
Once the buildings have been added, the Save button ![icon] must be clicked in order to continue on with the QUIC-URB simulation. Alternatively, when the City Builder is closed, a pop-up window will request that the user save changes.

Editing Building Dimensions
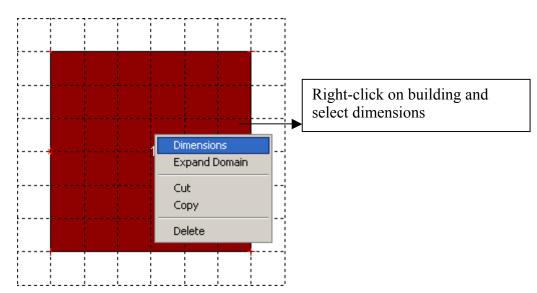
Dimensions of existing buildings can be adjusted by left-clicking one of the red vertices that define the outer extent of the building and dragging it to the desired building footprint. The building dimensions will automatically snap to the raster grid used by QUIC. This is shown in the figure below.
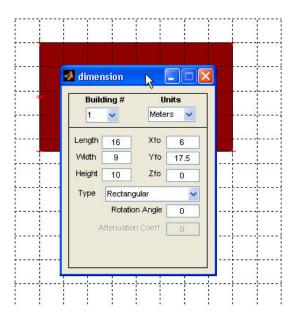
Buildings may be moved horizontally and vertically by left-clicking the red star that defines xfo and yfo for that building (the middle of the left-hand side of the building) and dragging it to the desired location on the grid. The building location will automatically snap to the raster grid used by QUIC. This is shown in the figure below.
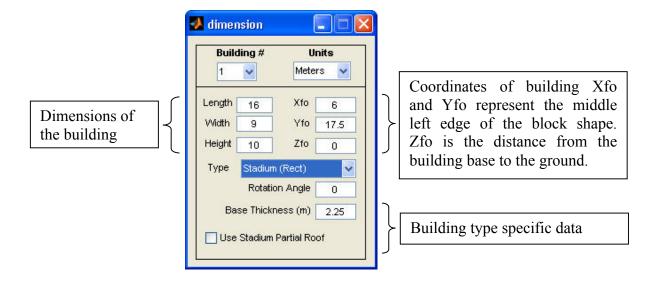
Alternatively, attributes of existing buildings can be edited by right-clicking the building and selecting "dimensions". This launches the Dimension Edit Box, where all building attributes may be adjusted. Building height, base height (zfo), and rotation angle (only available for pentagonal buildings) can only be adjusted using the Dimension Edit Box. This is shown below.

Right-click on building and select dimensions

Dimension Edit Box

Dimensions of the building

Coordinates of building Xfo and Yfo represent the middle left edge of the block shape. Zfo is the distance from the building base to the ground.

Building type specific data

Copy Building

To copy a building, right click on the building and select 'copy'. Then, at any other point in the domain, right click and select 'paste' to copy buildings from one location to another. This is shown in the figure below.

Grid Resolution

The grid resolution of the QUIC-URB modeling domain is specified in the text boxes on the upper right hand corner of the City Builder window. It is strongly recommended that the grid size should be set before creating buildings. If t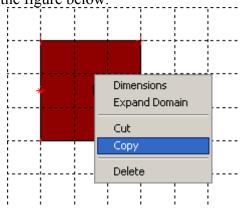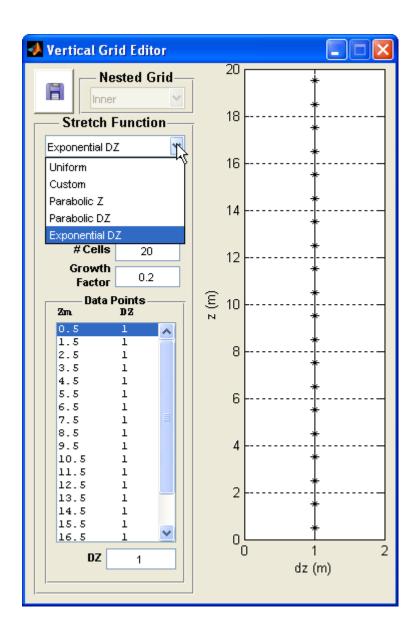he buildings are created first, and then grid resolution is changed, the buildings may not be resized optimally. Notice that the grid size can be different in the x, y, and z directions. For example, one may desire more resolution in the vertical and set this to 2 m, while setting the horizontal grid to be 5 m square. The default grid size is 1 meter. In addition the vertical grid does not need to be uniform throughout the domain. Selecting anything other than 'uniform' on the popup menu at the bottom of the domain panel launches the Vertical Grid Editor which allows the user to specify the function used to vary the size of the grid cells in the vertical direction. This GUI will be discussed in further detail in the next section.
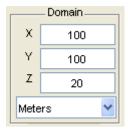

Vertical Grid Editor

There are several advantages to allowing the size of the grid cell to vary with height. It allows the user to make better use of resources because the fine resolution can be used where it is most needed (typically near the surface where there are strong gradients in the velocity field) and coarse resolution can be used in regions where the vertical gradients in the flow are small (typically at the top of the domain). Not only does this reduce the amount of RAM used in the simulation but it will also improve the QUIC-URB run time since it iterates over smaller arrays. The user can select from five different stretching functions: Uniform, Custom, Parabolic Z, Parabolic DZ, and Exponential DZ. Uniform simply forces all of the cells in the domain to be the same size. This is the default selection. Custom allows the user to manually input the grid sizes. This is the most flexible but also can be tedious to enter. The remaining three functions allow the user to specify the function with which the vertical grid size will vary continuously throughout the domain.
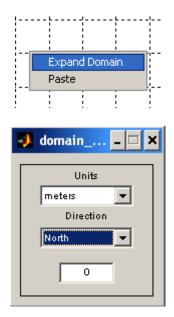
Domain Size

The domain size (number of grids or distance in the East-West (x), North-South (y) and vertical (z) directions) can be changed using the text boxes on the right hand side of the City Builder window. The units can be toggled between distance (meters) and number of grid cells using the pull-down menu selector.

You can also right click on empty space in the city builder map and add more grid cells to the north, south, east, or west of the domain. This is shown in the figure below.

Inner and Outer Grids
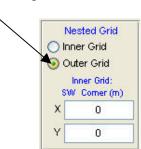
QUIC is normally run with a building-resolved grid. However, to cover larger areas, an outer grid option has been added. Here, the grid cell size is larger and buildings are not resolved. The outer grid could extend for tens of kilometers with 100 meter horizontal grid resolution, 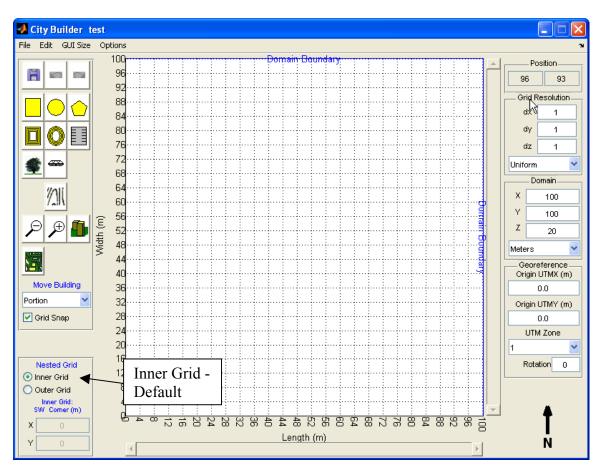for example. Buildings are not put on the outer grid; rather a roughness length parameterization is used instead. While buildings are not used on the outer grid, vegetation canopies (see the following section) may be used on the outer grid to simulate different land use characteristics over large areas. Note that a release of airborne contaminant on the inner grid will automatically be transported onto the outer grid (see QUIC-PLUME section).

When the City Builder is first brought up, it defaults to the inner grid.
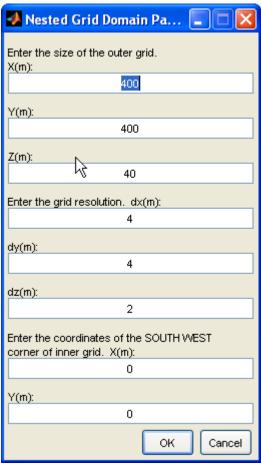
To specify an outer grid, one needs to:
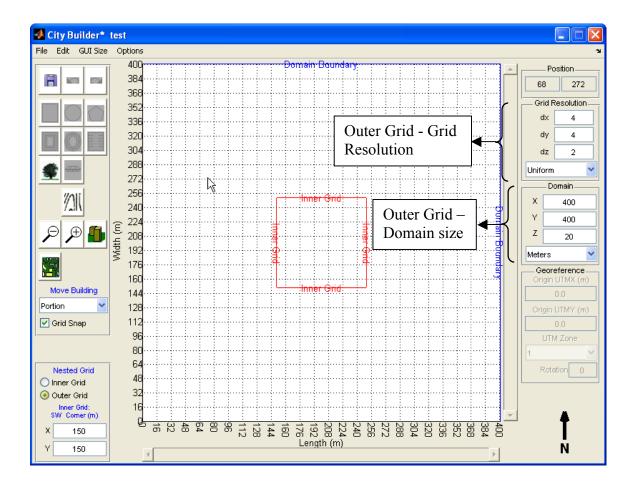
- First save the existing project on the inner grid using the 'save' button

- Now select the 'Outer Grid' Option

- This opens a window where in the outer grid parameters can be entered
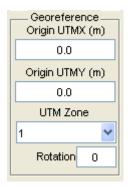
- Type in the appropriate parameters and press 'ok'
- This places an outer grid around the inner grid in the City Builder
- Various parameters of the outer grid such as the grid resolution and domain size can be now be seen in the City Builder

Geo-Referencing QUIC Domains

Since version 4.5, QUIC has had the ability to geo-reference domains through the controls on the lower right-hand side of the GUI shown below:
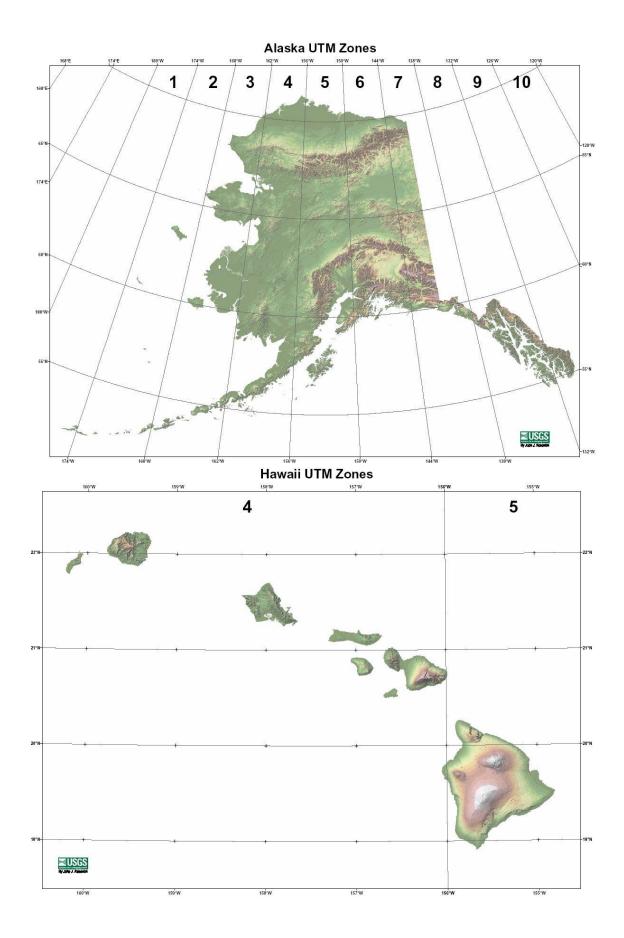
QUIC domains are geo-referenced using the Universal Transverse Mercator (UTM) system. The required inputs are the UTM zone, UTMX and UTMY locations of the inner grid origin, and domain rotation from true north (clock wise rotations of the domain are

considered positive angles). The GUI automatically calculates the UTMX and UTMY locations of the outer grid origin given the location of the inner grid, the relative location of the inner grid to the outer grid, and the rotation angle of the domain. The north arrow in the lower-right-hand corner of the GUI shows the direction of true north relative to the grid. Rotation angles can be between -45 and 45 degrees.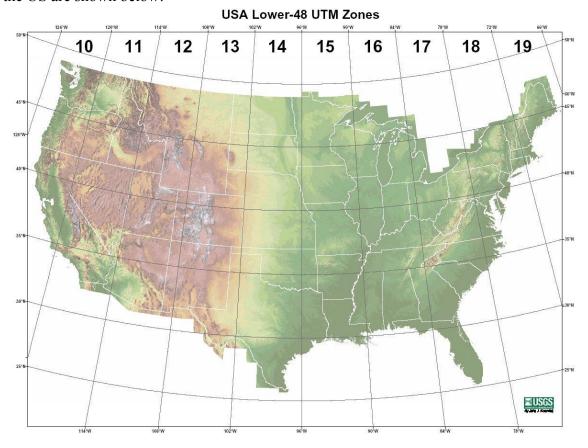 The user is encouraged to align the domain such that the majority of the buildings in the domain (or buildings of special interest within the domain) are aligned with the orthogonal grid used by QUIC.

UTM zones range from 1 to 60. The default UTM zone is 0 which is only a place holder since it is not within the range of actual UTM zones. The value of 0 informs the GUI that the QUIC domain has not been geo-referenced. Maps of the UTM zones corresponding the US are shown below:

USA Lower-48 UTM Zones

Alaska UTM Zones

Hawaii UTM Zones

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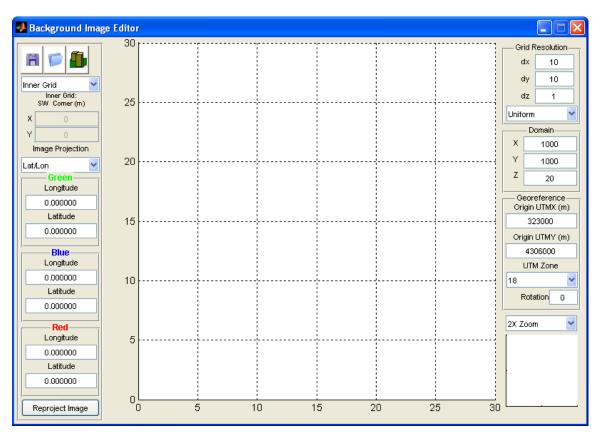
Add a Background Map
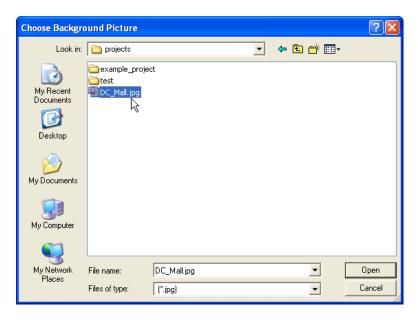
Background maps facilitate more accurate reproduction of urban areas.

Pressing launches the Background Image Editor.
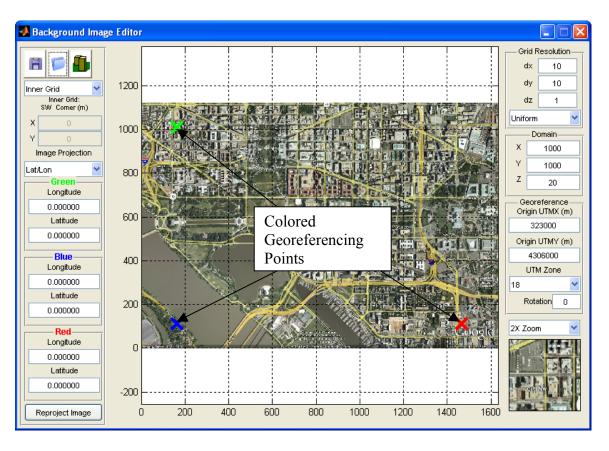
In older versions of QUIC (versions 5.5 and lower) adding a background image caused the GUI to resize the domain to correspond to the scaled background image. Later the image was displayed by stretching the image to fill the domain. This caused problems when resizing a domain because it would distort the background image to fill the new domain dimensions. The background image is now decoupled from the domain and is georeferenced. This ensures that domain changes will not affect the image so it will be an accurate representation of the region simulated.

Press the Open File button to browse for a jpg image file.

After selecting the desired file the image will be displayed in the axes in the center of the GUI.

Now that the background image has been loaded into the GUI the image is georeferenced by dragging the three colored X's over points on the image with known coordinates in either latitude and longitude or UTM. Another advantage of georeferencing the image, in addition to avoiding distortion problems due to resizing the domain, is that many images (such as those from Google Earth®) are displayed using latitude and longitude regardless of the coordinate system that they are using to display the cursor location in. Since QUIC alw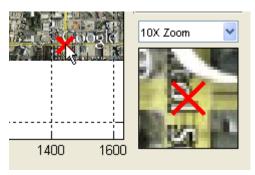ays uses UTM there can be a significant amount of distortion introduced by using an image displayed in lat/lon as if it were displayed in UTM. Thus domains produced with the new method will be a more accurate representation of the region than previous versions.

In order to georeference the image, left click on the three colored Xs and drag them to points with known locations. The chosen points should not be colinear. The zoom axes in the lower right-hand corner of the GUI allow the user to place the reference points with greater precision. Use the popup menu to select the zoom factor.
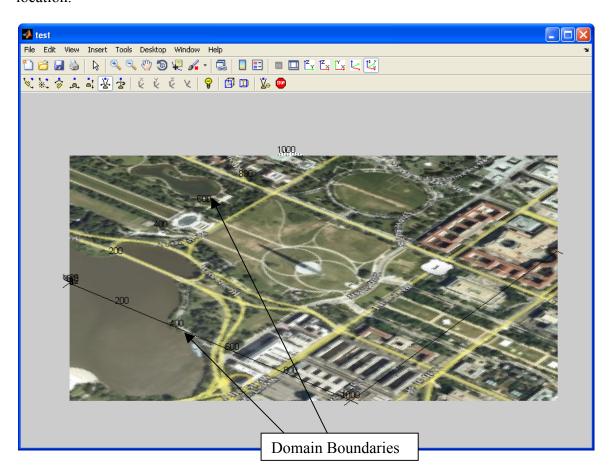
After the reference points have been dragged to the proper locations on the image the coordinates of each point should be entered in the edit boxes along the left-hand side of the GUI.
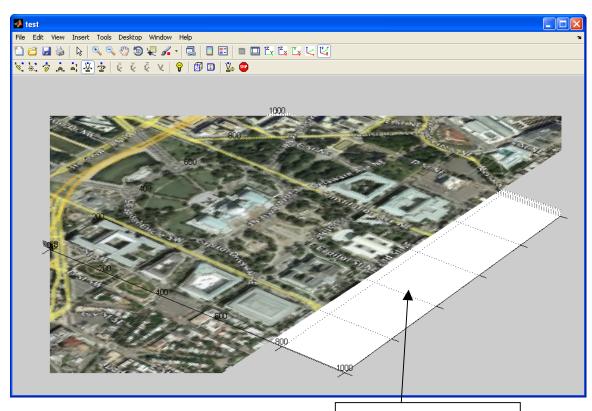
Once the coordinates for each of the domains has been entered, press the button in the lower left-hand corner of the GUI. This reprojects the

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image into UTM (if necessary) and the QUIC coordinate system. Now the image is ready to be displayed. You can view the back ground image by pressing the Plot 3D City button [icon]. Note that the 3D plot initially displays at an oblique angle. From this perspective you can see that the actual image in this example extends beyond the domain boundaries. This demonstrates the decoupling of the background image and the domain location.

Domain Boundaries

If the origin of the QUIC domain is shifted 2.5 km East of the previous value, the image automatically shifts to match with the new modeled domain. Note that the domain now partially extends beyond the limits of the background image.

Region of the domain not covered by the image

Elevation and Land Use Data

Pressing the Elevation and Land Use button will launch the Elevation and Land Use GUI shown below. Both elevation and land use data are optional. QUIC-PLUME can use the elevation data to account for terrain effects on dense gas dispersion. The land use data can be used to automatically extract vegetative and/or urban canopy data throughout the domain.
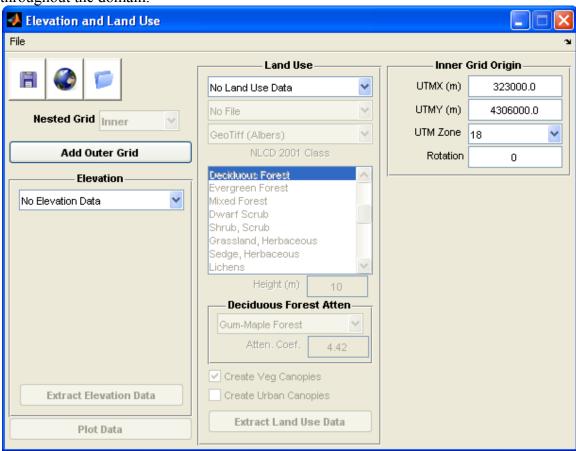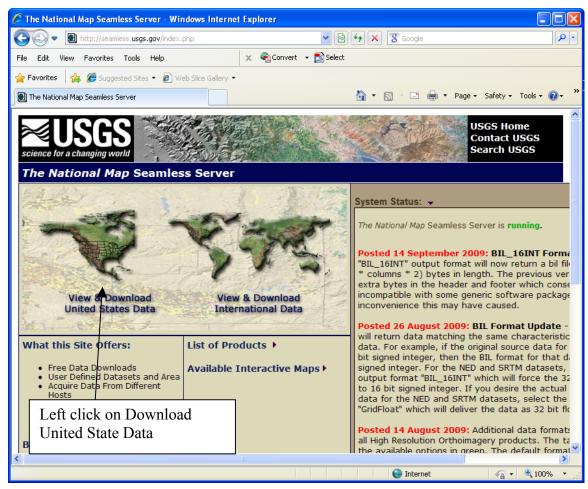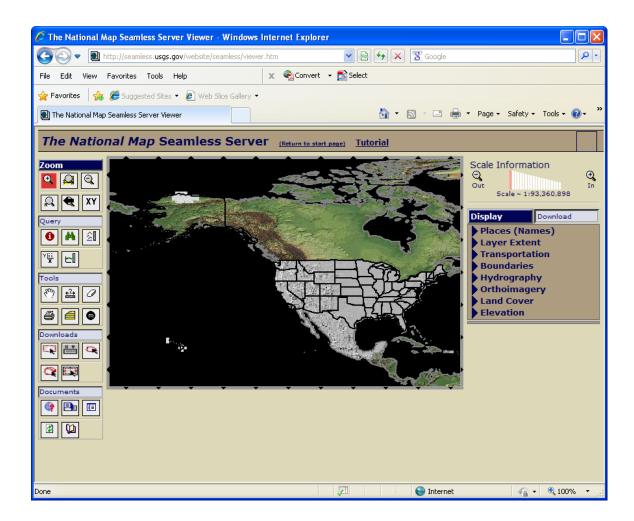

CAUTION: The user should be aware of the fact that land use in and around cities can and does change. The newest available data is from 2001. Some regions have experienced significant changes since then. So the user should exercise caution when automatically importing land use data. Also since the data was automatically generated using remote sensing techniques by groups who did not have this particular application in mind, it is far from perfect particularly for fine scale inner grids. Some regions that for the purposes of a QUIC simulation should be classified as vegetative canopies may be classified as urban land cover. The urban land cover classes can be particularly misleading since they are based on the percentage of the surface in the cell that is covered by manmade materials. So a "High-Intensity Developed" cell might be used for a parking lot or road as well as for a skyscraper. The land use data is most useful for outer grids, which can cover a large area and only really need to get a general sense of the effects of land use on the transport and dispersion.
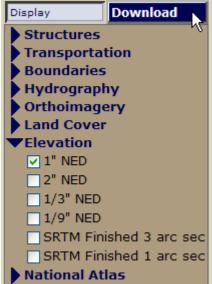
Press the internet button to launch the USGS Seamless Server web site in the default web browser.
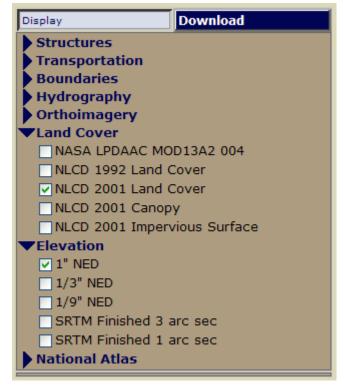
Clicking on View and Download United States Data will bring up the National Map Seamless Server as is shown below:

Now click on the download button on the right-hand side of the page.

Select the desired elevation data resolution (if you wish to include terrain effects on dense-gas dispersion) and the NLCD 2001 Land Cover data (if you wish to import canopy data).
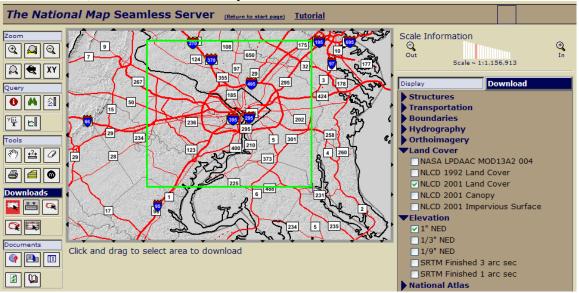
Use the magnifying-glass tool (found on the left-hand side of the page) to drag a region on the map and zoom in on the region of interest. Now you can graphically select a rectangular region that you would like to download data for by pressing found in
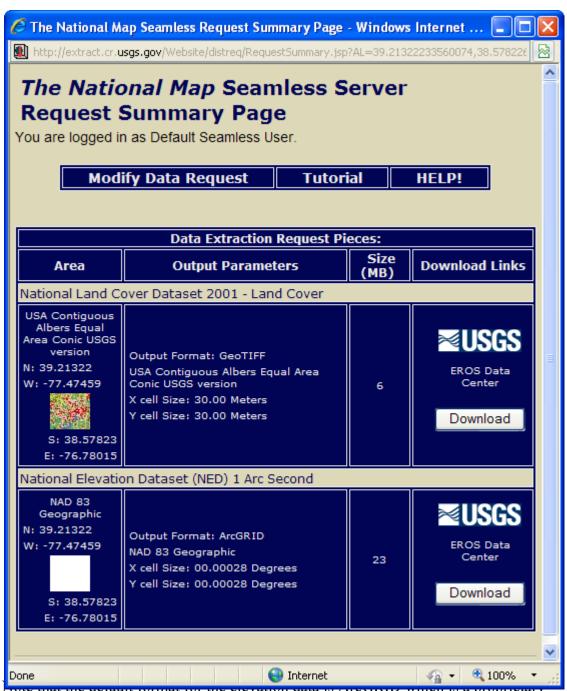
the downloads section on the left-hand side of the page or you can use one of the other tools to use a different method select the region.

You may want to download two different elevation resolutions, one for the inner grid and another for the outer grid, to get the necessary resolution for the inner grid while keeping the size of the file as small as possible to speed up the extraction process.

Note: Make sure that you select a region that is significantly larger than the QUIC domain. This is because the elevation data is projected in Lat/Lon and the land use data is projected in USA Contiguous Albers Equal Area Conic. Since the output is a 2D array aligned with the corresponding coordinate system the selected regions will not cover identical regions. Also note that while there are several different choices in resolution of elevation data, the land use data always has a 30 m resolution.
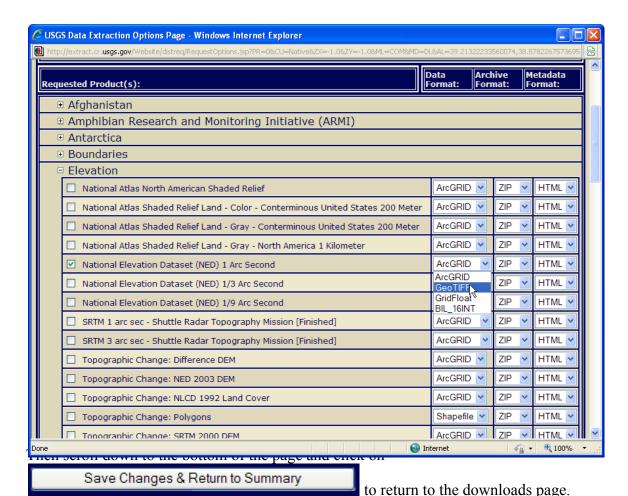
After selecting a region to download the data (indicated by the green box above) the Seamless Server will open a new window.
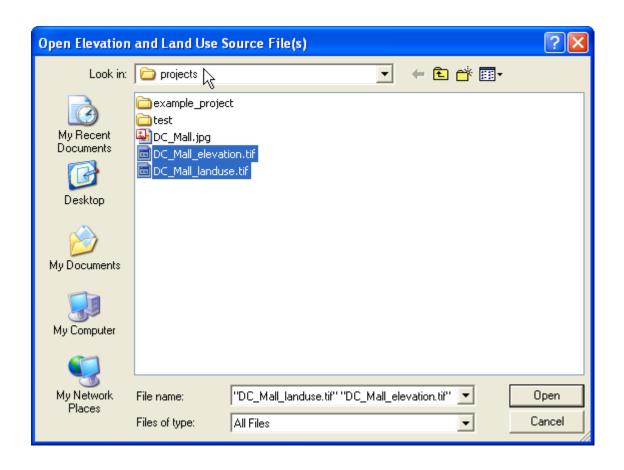
Note that the default format for the elevation data is ArcGRID which is a proprietary format used by ArcGIS® and cannot be opened using the Mapping Toolbox in Matlab®.

Instead you will need to click on **Modify Data Request** near the top of the page. This will open the Request Options page in the new window. Scroll down to the selected National Elevation Dataset (NED) resolution and change the data format to GeoTIFF.

Then scroll down to the bottom of the page and click on

 to return to the downloads page.

You are now ready to download the elevation and land use to your computer. Simply click on the download button for the desired data set and the server will extract the data and prompt you download the file. Depending on your browsers security settings you may have to tell it that the file is okay to download. Also depending on the size of the file and the amount of traffic on the server at the time that you are attempting to download the data, it may take a while to extract the data and send it to you.

Now that you have downloaded the data to your computer, press to browse to the location of the elevation and land use GeoTIFF files that you just downloaded. You can select multiple files to import at the same time. Use the <shift> and <control> or <command> (depending on your OS) to select multiple files.
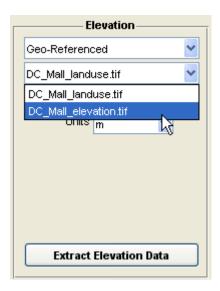
Adding Elevation Data

Elevation data can be added with two different ways: A constant slope over the domain and georeferenced data extracted from a file.

To set a uniform slope across the domain select "Uniform Slope" in the popup menu at the top of the Elevation panel. Then enter the gradient vector direction (measured from true north which is not the y-direction in QUIC if you have a rotated domain) and the grade in percent. Then press the "Generate Elevation Data" button to populate the elevation arrays.

To extract elevation data from a file select "Geo-Referenced" in the popup menu at the top of the Elevation panel. If the next popup menu says "No File" then you need to follow the instructions above to download data from the USGS Seamless Server and open the files in the Elevation and Land Use GUI. Once some files have been specified for use in the GUI, select the desired elevation file from the list in the second popup menu in the Elevation panel

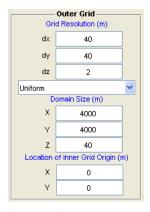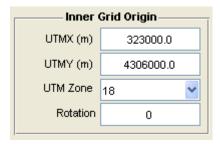The default file format for elevation files is GeoTIFF projected in Lat/Lon coordinates, which is what you will get from the USGS server. The default units are meters which is also what is returned by the USGS server by default. Once the proper file has been selected, choose the grid (inner, outer, or both) to which you wish to extract the data.

If you have not yet created an outer grid but wish to do so now you can press the "Add Outer Grid" button to add an outer grid to your project from the Elevation and Land Use GUI. Selecting "Outer Grid" in the popup menu will make the outer grid controls on the right-hand side of the GUI visible.
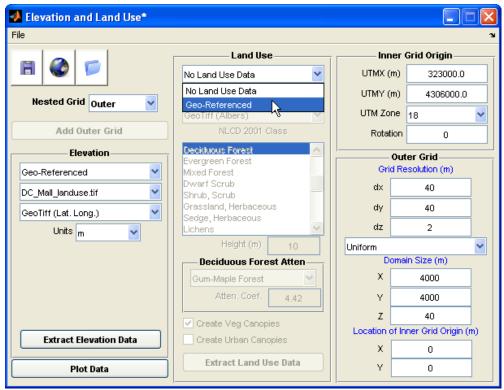
You can also georeference the QUIC domain or change the location of the inner grid's origin using the controls in the upper right-hand corner of the GUI. The georeferencing of the outergrid is coupled to the georeferencing of the inner grid and the location of the inner grid relative to the outer grid.
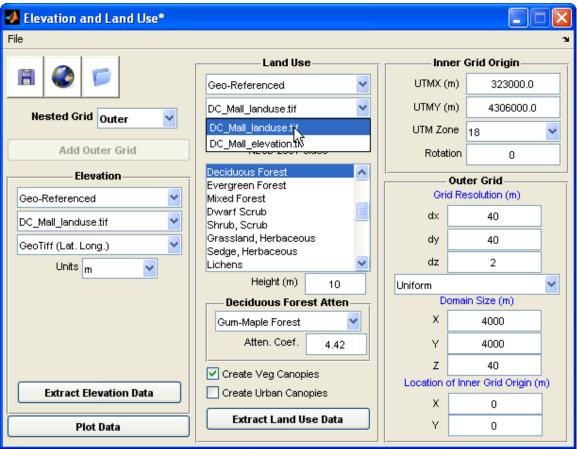
Once the proper file and format have selected and the domains have been georeferenced, press the [Extract Elevation Data] button located at the bottom of the Elevation Panel to extract the elevation data from the file for the selected domain(s). Depending on the resolution of the file this may take a while.

Adding Land Use Data

Land use data can only be added by extracting georeferenced data from a file. To add land use select "Geo-Referenced" in the popup menu at the top of the Land Use Panel.

This will activate all of the other land use controls in the panel. Next select the desired file with the land use data in the second popup menu from the top.

The default file format for land use is a GeoTiff using the USA Contiguous Albers Equal Area Conic projection. This is the default for this data on the USGS Seamless Server. Below the popup menus at the top of the panel you will find the library of NLCD 2001 land use classes listed by name. Included with QUIC is a default library which associates each land use class with a corresponding canopy height and a canopy type from the library of attenuation coeff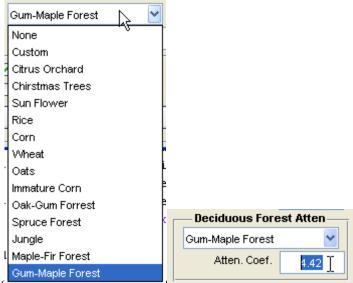icients (Cionco 1978). A customized land use library is saved inside of each project so the user is allowed the flexibility to modify the various canopy parameters for as many land use classes as they wish without modifying the default land use library. The height of the canopy can be modified using the height edit box and the attenuation coefficient can be modified by either selecting a canopy type in the popup menu or changing the value in the edit box.

Before you extract the land use data you need to decide which classes to include. The urban land use classes are denoted as being "developed", checking the "Create Urban Canopies" checkbox includes the urban land classes in the generation of the height and attenuation coefficient arrays.
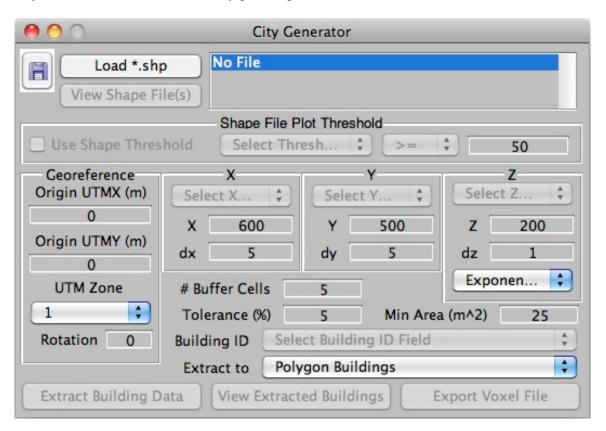

All other land classes are included in the "Create Vegetative Canopies" check box. Note that you can effectively remove the contribution of a single land use class by changing its height to '0'. As was mentioned above, care should be taken when using land use data, due to inaccuracies in the automatically generated database and old data that has since changed in urban areas. In general, the urban canopies should not be included for an inner-grid domain since the buildings are explicitly resolved but should be included for outer grid domains. Now that the land use library has been modified as necessary and the file has been selected, you are ready to extract the land use data from the file. To do so simply press the [Extract Land Use Data] button. QUIC saves the customized land use library, the array of land use classes, the array of canopy heights, and the array of canopy attenuation coefficients. This is done so that once the land use data has been extracted once the library that converts the land use data into canopy heights and attenuation coefficients can be modified later and the land used data can be converted into new canopy height and attenuation coefficient arrays without loading the land use file. Simply modify the land use library as desired and press the [Extract Land Use Data] button again to convert the saved land use data into new canopy height and attenuation coefficient arrays.

Note: The user defined canopies from Citybuilder will be used instead of the land use based canopy arrays wherever applicable. This provides a method for correcting inaccuracies in the land use data. A region of extra tall canopies can be added (e.g. to model extra tall buildings in the central business district on an outer grid) or land use canopies can be effectively be removed by drawing out a canopy with a height less than half the surface level vertical grid size height (useful for surgically removing regions that have been developed since the database was created).
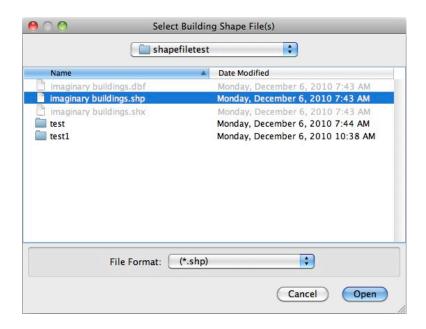
Importing Shape Files

QUIC can import ARC GIS shape files directly into polygon buildings or a 3D building array that is useable only by QUIC-CFD. If a 3D building database is available this will greatly speed up the process of generating a new QUIC domain. QUIC requires that the shape files be in UTM with all dimensions (x, y, and height of buildings) in meters. The
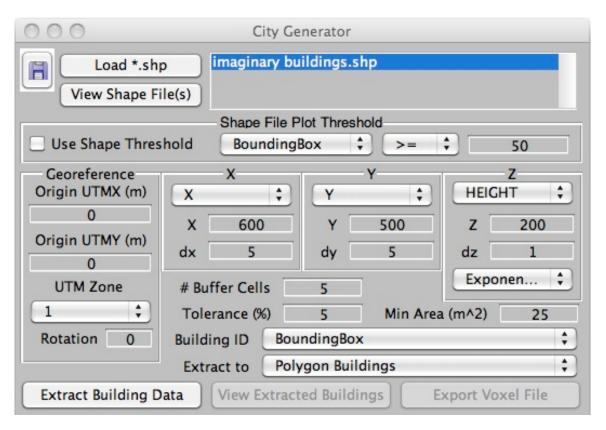
City Generator Tool is accessed by pressing the [icon] button.

To import a 3D shape file first load the shape file into the GUI by pressing the Load *.shp button and navigating to the desired shape file(s).
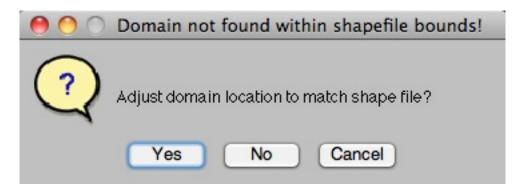
Once the shape file has loaded into the GUI it will show up in the list of available shape files in the upper-right hand corner of the City Generator GUI.
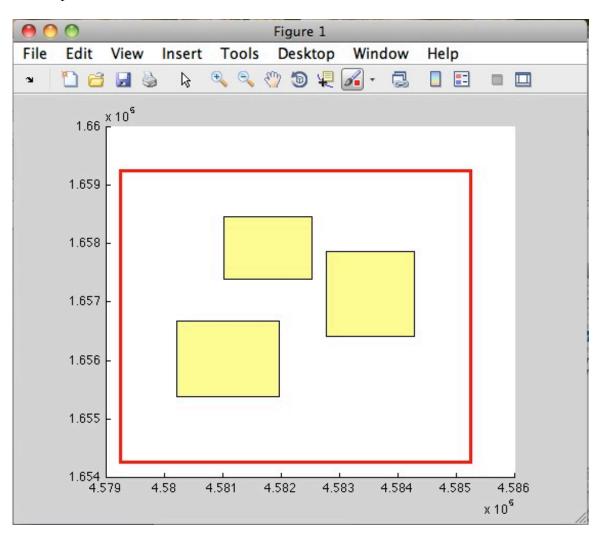
Note that once a shape file has been read into the GUI more controls are enabled. The user can now press to view the buildings in the shape file relative to the QUIC domain. If the QUIC domain has not been georeferenced or the

buildings in the selected shape file(s) are not within the extent of the QUIC domain the user will be prompted if they wish to center the QUIC domain on the shape file when attempting to plot the shape file or extract the building data.

A plot of the shape file buildings (yellow polygons) and QUIC domain (red box) with then be produced.

The 'Use Shape Threshold' option is intended to speed up plotting of the shape file by down selecting the polygons in the shape file that are plotted by a user defined threshold. This can be particularly important in detailed building databases that cover large portions of a city, where it may take a great deal of time to plot each individual polygon.

IMPORTANT NOTE: Before extracting the building data the user must verify that the appropriate fields are selected for X (UTMX of polygon nodes), Y (UTMY of polygon nodes), and Z (building height). The GUI searches the available fields for appropriate selections but it may not select the proper field since field names are not universal in shape files.

Press [Extract Building Data] to extract the shape file data into QUIC polygon buildings or a 3D building array for use in QUIC-CFD.

'# Buffer Cells' sets the number of cells around the perimeter of the domain that are to be left empty. This means that buildings that have a portion of their footprint that extend our in the buffer area will be omitted from extraction. If a building has been omitted from extraction then adjust the domain to include that building and press [Extract Building Data] again.

'Tolerance' sets the tolerance level at which the GUI will check the area and perimeter of a polygon to see if it is either a rectangular or elliptical building. Only completely solid buildings are translated to simple QUIC building geometries.

'Min Area' sets the threshold for the polygons that will be extracted. Polygons and holes in polygons must have an area larger than this minimum area to be extracted.

The 'Building ID' pop-up menu selects the field that identifies the various polygons that make up an individual building. This information is used by QUIC to properly account for the wakes of stacked buildings.
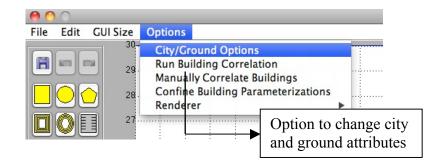
The 'Extract to' pop-up menu is where the user decides to extract to either polygon buildings for use in QUIC-URB or a 3D building array for use in QUIC-CFD.

A 3D view of the extracted building data can be seen by pressing [View Extracted Buildings].

City Builder Options

Select <Options> on the City Builder pull-down menu to change City Builder viewing options.
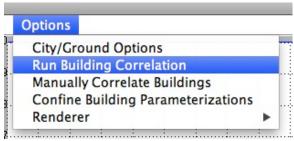
Option to change city and ground attributes

The City Builder Options window controls the color and the information displayed. Building color, ground color, and transparency is specified here. Building numbers and axes can be turned on and off.

- click Apply or OK to accept changes.

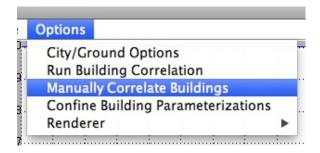Note: The output of VIS Gui is also controlled by this pop-up window.

Run Building Correlation

Select the 'Run Building Correlation' from the options pull down menu. The run building correlation option looks for buildings that are touching and groups them together through a building group id.

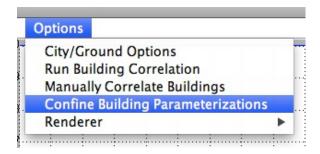## Manually Correlate Buildings

Select the 'Manually Correlate Buildings' from the options pull down menu. This option provides the user the capability of manually grouping buildings together, even those that are not touching. This option is not functional in the present version and will be included in the future versions of QUIC
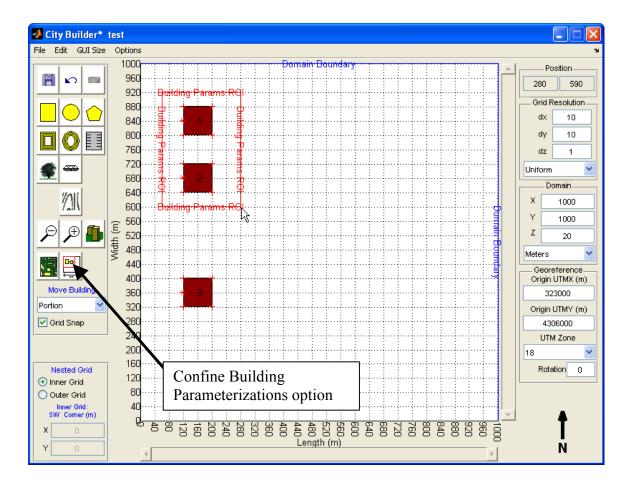
Confine Building Parameterizations

Select the 'Confine Building Parameterizations' from the options pull down menu. This option provides the user the option of applying the building flow parameterizations to only selected buildings, i.e., those within a user defined rectangle. On selecting the option, an icon appears in the main City Builder window as shown below.
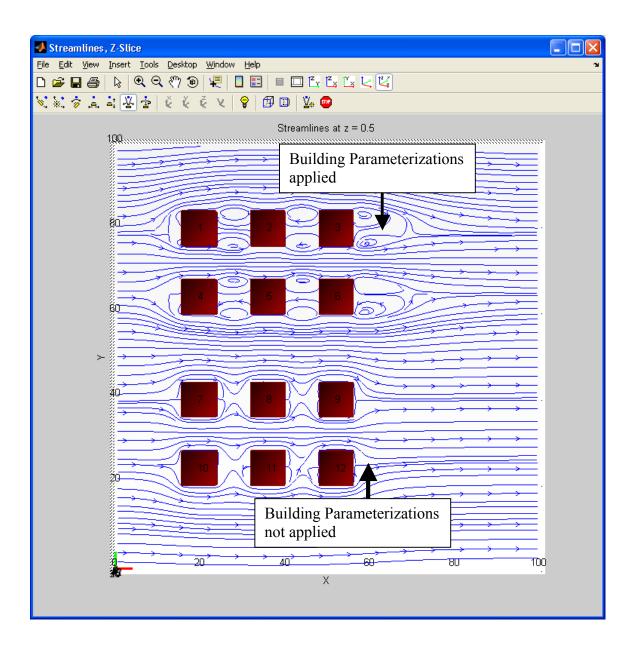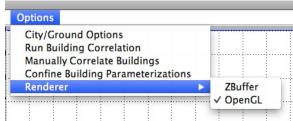
Press this button and with the cursor select an area around the buildings where you would like to confine the parameterizations. This is has been shown below:

The figure above shows the region over which the building parameterizations are confined. Building flow parameterizations are not applied to the other buildings and only the initial flow field is utilized. The effect of turning off the building parameterizations can be seen in the plot below.
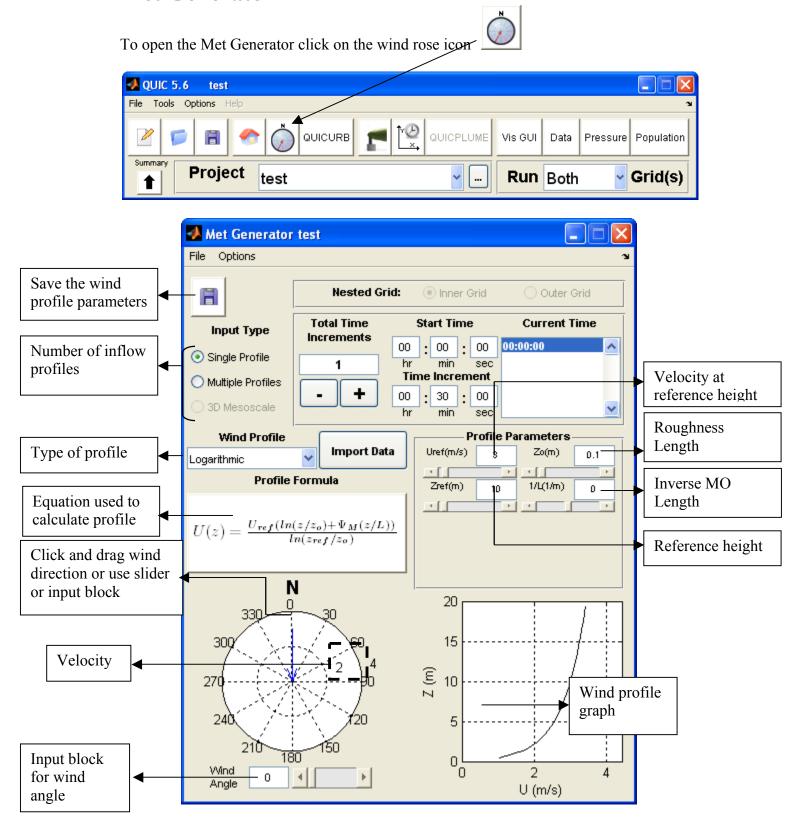
Renderer

The default renderer for Citybuilder is OpenGL. This allows the GUI to use transparency when plotting the buildings so the background image can still be seen below them. You may want to use ZBuffer instead because it plots significantly faster and is less prone to visualization bugs. Some graphics cards will not display the 2D city map properly. If you are experiencing visualization issues in Citybuilder, change the renderer mode to ZBuffer.

Met Generator

To open the Met Generator click on the wind rose icon

Save the wind
profile parameters

Number of inflow
profiles

Type of profile

Equation used to
calculate profile

Click and drag wind
direction or use slider
or input block

Velocity

Input block
for wind
angle

Velocity at
reference height

Roughness
Length

Inverse MO
Length

Reference height

Wind profile
graph

Profile Formula

$$U(z) = \frac{U_{ref}(ln(z/z_o) + \Psi_M(z/L))}{ln(z_{ref}/z_o)}$$
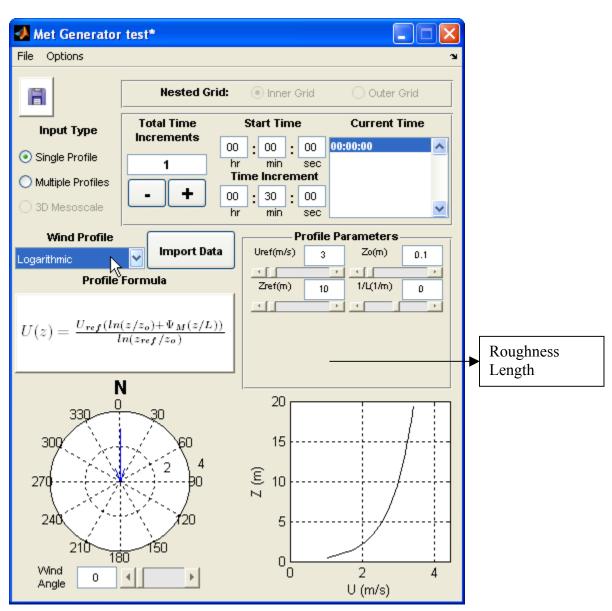
- The inflow conditions are specified here. The wind direction is specified through the compass and arrow. The wind speed is a function of height and can be specified as a power-law, log-law, urban canopy, or user-specified profile.
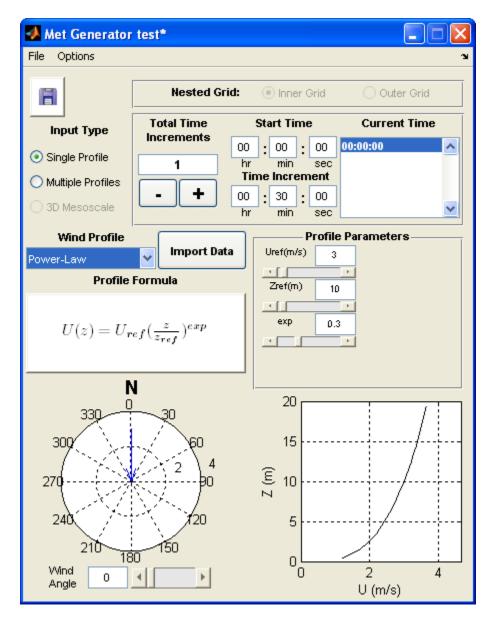

Wind Profile Types

Logarithmic Profile

The logarithmic wind profile equation is shown when Logarithmic is selected.

Roughness Length
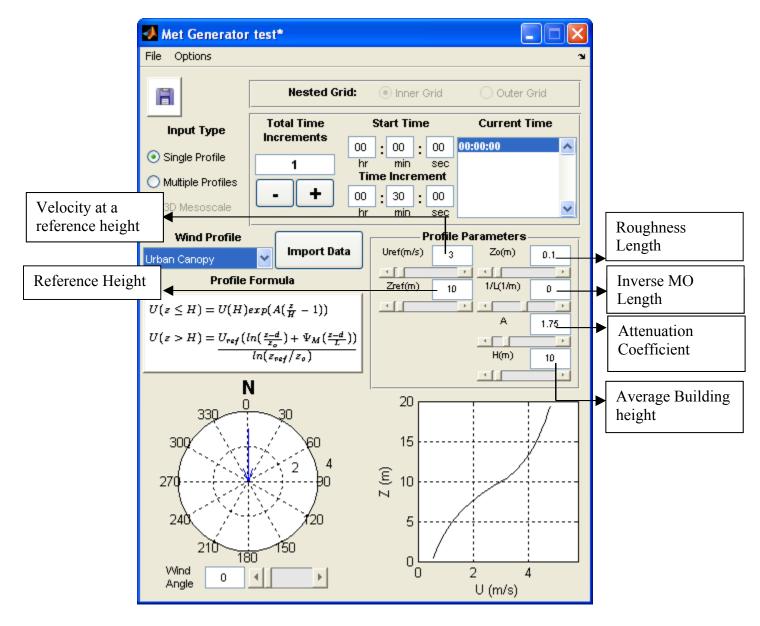
Power-Law Profile

The screenshot below shows the power-law profile parameters.

The wind profile type is selected through the "Wind Profile" pull-down menu. The profile parameters box to the right changes for each wind profile type.
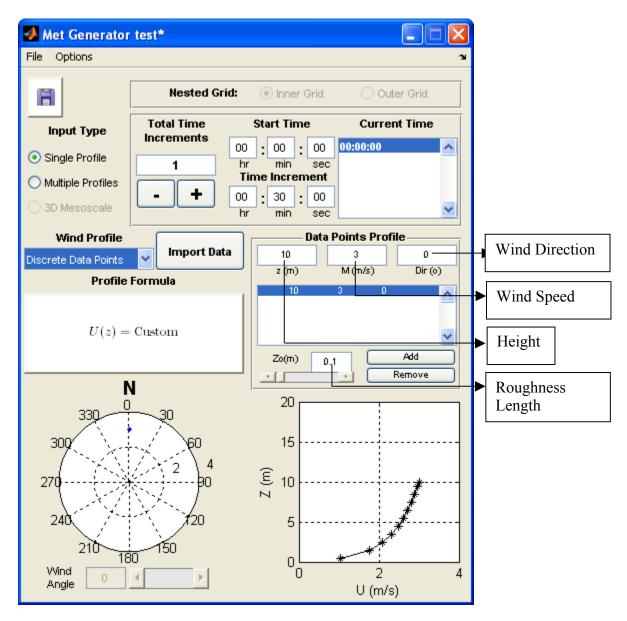
Urban Canopy Profile

In the screen shot below the Urban Canopy Profile has been selected. This profile represents the area-average impact of buildings (or vegetation) on the flow. The region of low wind speeds below average canopy height H is typical of winds that have been slowed by buildings and vegetation upstream of the point of measurement. This profile uses a different equation for winds above and below the reference height (H). As seen in the screen shot this profile requires a lot more parameters than any of the other profiles. It is possible to create a profile that is discontinuous at H, thus care should be taken to avoid this situation, as it will affect the accuracy of the results.

Discrete Data Points (User-Specified) Profile

A text box will come up where you can hand type in information. Using this profile it is possible to enter profiles with directional shear (i.e., wind direction does not have to be constant with height). Users are cautioned against running the model with large amounts of directional shear below building height as this will likely produce unrealistic results.

In the text box shown in the figure above, enter the value of wind speed at a given height. The wind direction and roughness length z0 can also be specified.

If the user has the values of all three components of velocity at a given height, the user can input them manually by choosing the vector option as shown below. It should be noted, however, that QUIC-URB does not currently use the vertical velocity components
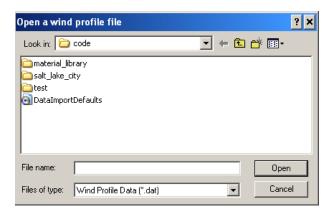
when initializing the wind field. The profile is extrapolated from the lowest data point to the ground using a logarithmic profile with a user specified roughness length (z_0).

Import Data
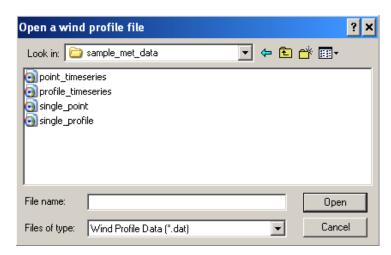
One can also directly import a data file in a four column space delimited format: time (decimal hours), height (meters), wind speed (meters per second), wind direction (degrees). To do so

- select "Import Data" **Import Data**

This opens a window titled 'Open a Wind Profile' as shown below

Open the folder titled 'sample_met_data' in the main QUIC folder. This folder has sample velocity profiles.
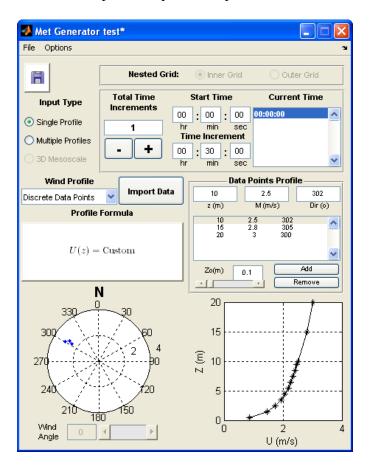
- select a wind profile data file in the format mentioned in the above paragraph

- press "Open"
- The GUI will automatically determine if the imported data file constitutes a profile or single point measurement.
- If the data is for a single point measurement, the GUI will prompt the user to select a profile type as seen below. Enter the number corresponding to the desired profile type and press "OK".

- Figure below shows a sample wind profile imported into the Met Generator

Multiple Profiles

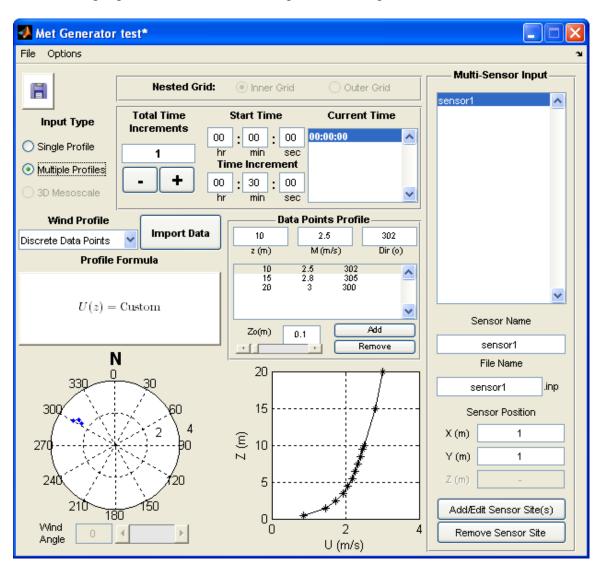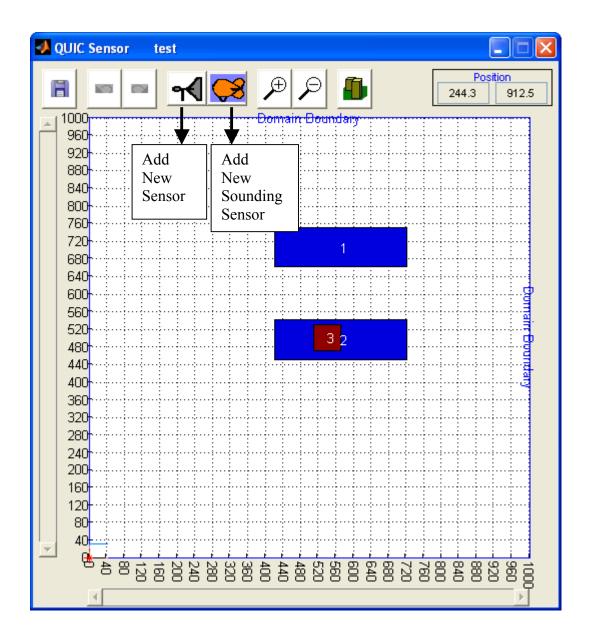To add multiple profiles, choose the 'Multiple Profiles' option as shown.

QUIC-URB uses quasi-3D Barnes mapping to interpolate the initial wind fields between sensors. This option is useful for modeling real cities that have multiple wind sensors in different parts of the city. Sensors can be placed in the modeled city by choosing the 'Add/Edit Sensor Site(s)' Add/Edit Sensor Site(s) option.
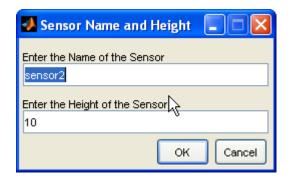
Clicking this option brings up the 'QUIC Sensor' Window as shown.

The QUIC Sensor window has the 'Add New Sensor' (single point measurement with an extrapolated profile) and 'Add New Sounding Sensor' (profile measurement with logarithmic extrapolation to the ground) options as shown. To place a sensor at a particular location, click in the appropriate icon and place the sensor with the cursor by clicking at the desired location as shown.

This brings up a pop up window as shown. In this pop up wind enter the sensor name and the height of the sensor and press 'ok'. This places the sensor at the desired location. This is shown below.
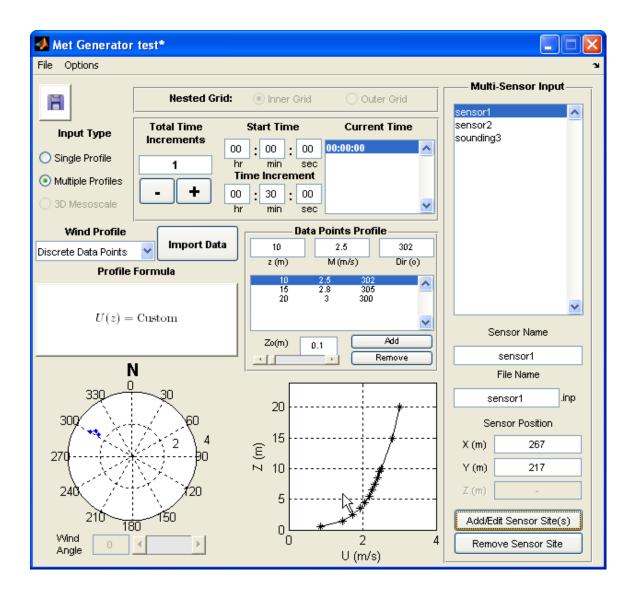
To place a sounding sensor, follow the same procedure and a pop up window will appear. In this pop up window enter the sensor name and press 'ok'. This will place the sounding sensor at the desired location.

After all the sensors are placed, click the save button before exiting.
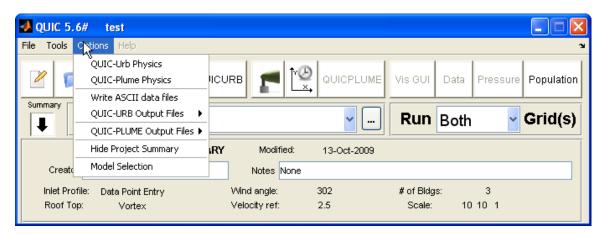
Once the user exits the QUIC Sensor window, he / she is directed back to the MET Generator. Here, select the appropriate sensor and enter the wind parameters.

To delete a sensor, use the 'Remove Sensor Site' option.

QUIC-URB Physics Options

Several empirical algorithms used by the QUIC-URB wind model can be changed through the Physics Options pop-up window. On the main QUIC-GUI window select <Options> <QUIC-URB Physics>.

This launches the QUIC-URB Physics options GUI as shown below:

Rooftop Algorithm

There are three choices for the rooftop algorithm: original Rockle (a free-slip boundary condition), logarithmic (a no-slip boundary condition), and recirculation (a rooftop vortex). The recirculation option is recommended.
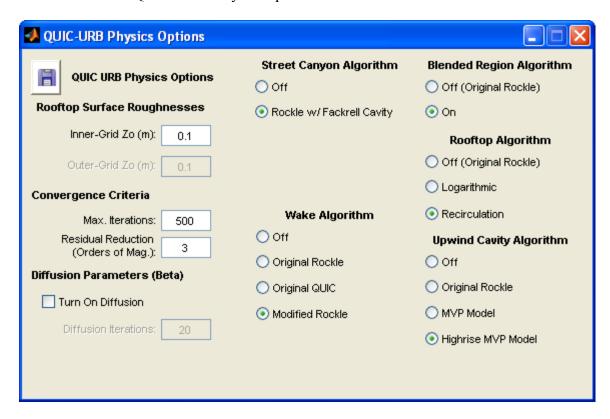
Street Canyon Algorithm

The street canyon vortex can enabled or disabled. The street canyon vortex algorithm uses the Fackrell cavity length parameterization which limits the effect of aspect ratio on the length of the downwind cavity.

Upwind Cavity Algorithm

The upwind cavities can either be disabled (off) for all buildings or the user may select from one of three parameterizations: Original Rockle, an ellipsoid region of zero velocity; Modified Vortex Parameterization (MVP), inserts a vortex and velocity retardation region but does not account for the effect of tall buildings on the extent of these regions; and Highrise MVP, similar to MVP but limits the size of the vortex for tall buildings. All upwind cavity parameterizations are only applied in front of rectangular shaped buildings (basic rectangular, rectangular stadium, parking garage) which have a face that is within 10° of being perpendicular to the approach flow. The Highrise MVP model is recommended.

Blended Region Algorithm

Formerly known as the intersection algorithm, this causes regions near street canyons to interpolate the flow around them. It is recommended that this be turned on.

Wake Algorithm

The wakes and downwind cavities behind buildings can either be turned off or the user can select from one of three parameterizations. The primary difference in the parameterizations has to do with the definition of the characteristic dimensions of the building which in turn determine the size of the wake. A further description of the difference in the algorithms can be found in Nelson et al. (2008). The modified Röckle algorithm is recommended.
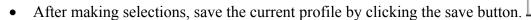
Convergence Criteria

The maximum number of iterations to perform to solve the Poisson equation used for mass conservation. This forces the code to stop even if the residual convergence criterion has not been reached. The recommended maximum number of iterations is between 500 and 1000.

The order of magnitude reduction in the residual to reach convergence. Three orders of magnitude reduction is recommended. Smaller problems generally require fewer iterations to converge.

Diffusion (Beta)

This option imposes the diffusion operator on the velocity field. This attempts to mimic the effects of turbulent diffusion on the mean flow field. The number of iterations determines how many times it is implemented. This option is experimental and as such is turned off by default.

- After making selections, save the current profile by clicking the save button.

QUIC-URB Input Files

The City Builder and the Met Generator sub-GUI's create the following input files for QUIC-URB:

List of files

Note: the *.proj* and associated input files can be modified outside of the QUIC-GUI as long as the parameters are chosen properly and the format is kept the same.

Running QUIC-URB

Once the building layout and inflow wind conditions have been defined, the QUIC-URB code can be run (if the parameters are not specified, the QUIC-URB button will be deactivated).

- Select the QUIC-URB icon. The light bulb indicates that QUIC-URB is running and the wind fields are being computed.

When the light bulb disappears, the QUIC-URB model has finished running. The computed wind fields can be used as input to the QUIC-Plume dispersion model, the QUIC-Pressure code, or can be visualized with the Vis-GUI. Refer to the Vis-GUI section for visualization options.
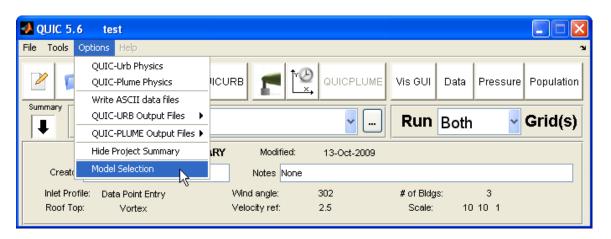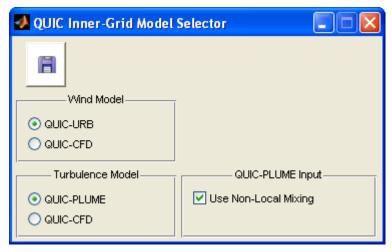
QUIC-CFD

QUIC-CFD

QUIC-CFD is a simplified computational fluid dynamics model that uses the QUIC-URB input files and produces a steady-state 3D mean wind field. It can be used in the place of QUIC-URB to produce the 3D wind field used by QUIC-PLUME. QUIC-CFD is faster than most CFD codes, but not as fast as QUIC-URB. While it is slower than QUIC-URB it can more easily handle complex geometries since it uses the governing equations instead of empirical parameterizations to produce the building effects on the flow field.
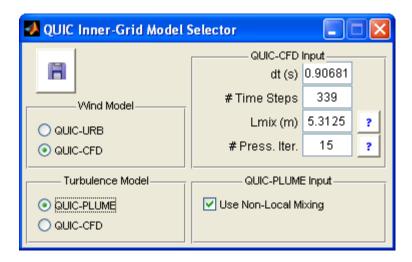
Model Selection

From the 'Options' menu at the top of the Main GUI choose "Model Selection":

By default QUIC uses the QUIC-URB wind solver to produce the wind field for QUIC-PLUME. Note also that the default turbulence model used is the one inside of QUIC-PLUME and that the non-local mixing option in QUIC-PLUME's turbulence model is turned on.

By clicking on the QUIC-CFD radio button, the user can choose to produce the wind field using QUIC-CFD:

When QUIC-CFD is selected the QUIC-CFD Input panel becomes visible (see above). The GUI will automatically generate values for these parameters based on the wind speed, the grid cell size, the size of the domain, and the average building height. Below is a list of the parameters and a brief description of each.

- dt - the CFD model time step (forced to satisfy the Courant condition).
- # Time Steps - the number of time steps used to allow the model to converge on a steady state solution.
- L_{mix} – the maximum allowable turbulent mixing length (based on the average building height)
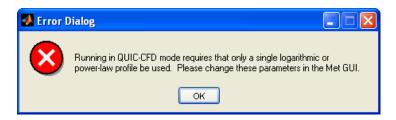- # Press. Iter. - the number of pressure iterations performed for each time step.

When running QUIC-CFD, the user has the option of using the turbulence fields produced by QUIC-CFD or using the default turbulence model inside of QUIC-PLUME. If the "QUIC-CFD" turbulence model option is selected, the non-local mixing option disappears in the GUI as this option is only available to the QUIC-PLUME turbulence model.

Note that selecting the "QUIC-CFD" turbulence model when the "QUIC-URB" wind model is selected will cause the GUI to automatically switch the wind model to "QUIC-CFD".

Pressing in the QUIC Model Selector GUI will save the model parameters to the appropriate input files in the project folder and the "QUIC-URB" button on the Main GUI will change to "QUIC-CFD":

NOTE: QUIC-CFD is limited to either a logarithmic or power-law inflow profile and cannot use multiple profiles within the domain. Multiple wind profiles in time are allowed, however. If you select the QUIC-CFD model when you have multiple sensors or are using the urban canopy or data points profiles you will receive the following message:

You then need to return to the Met Generator GUI and change the appropriate wind profile parameter settings.

Running QUIC-CFD

Once the building layout and inflow wind conditions have been defined, the QUIC-CFD code can be run (if the parameters are not specified, the QUIC-URB button will be grayed out and deactivated).

Press the QUIC-CFD icon. The light bulb indicates that QUIC-CFD is running and the wind fields are being computed.

You will notice that the GUI actually runs QUIC-URB (although without going through any iterations with the SOR solver) before it runs QUIC-CFD. This is because QUIC-CFD uses the QU_celltype.bin file produced by QUIC-URB to define the building cells in the domain. QUIC-PLUME will also need the QP_buildout.inp file produced by QUIC-URB if the QUIC-CFD turbulence model is not selected.

When the light bulb disappears, the QUIC-CFD model has finished running. QUIC-CFD automatically produces its own pressure data which can be visualized in the Pressure GUI. The winds can be visualized in the Vis GUI similarly to the wind fields produced by QUIC-URB.
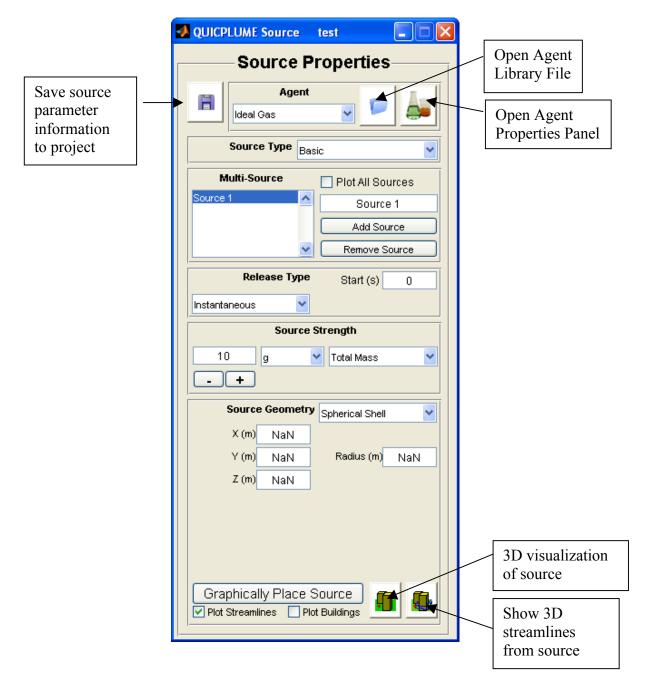
QUIC-PLUME

QUIC-PLUME Source Parameters

- To open the QUIC-PLUME Source Setup window click on the smoke stack icon.

- The source type, the release location, the size of the release, the release duration, and the material and associated properties are set here.
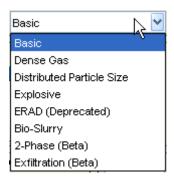
Save source parameter information to project

Open Agent Library File

Open Agent Properties Panel

3D visualization of source

Show 3D streamlines from source

Agent Type

The artificial agent library is included in the standard release of QUIC. This library includes six different agent types with various properties which can be used in QUIC-PLUME. They are shown below. An Official Use Only agent library with actual agent properties is available for users who meet the release requirements.
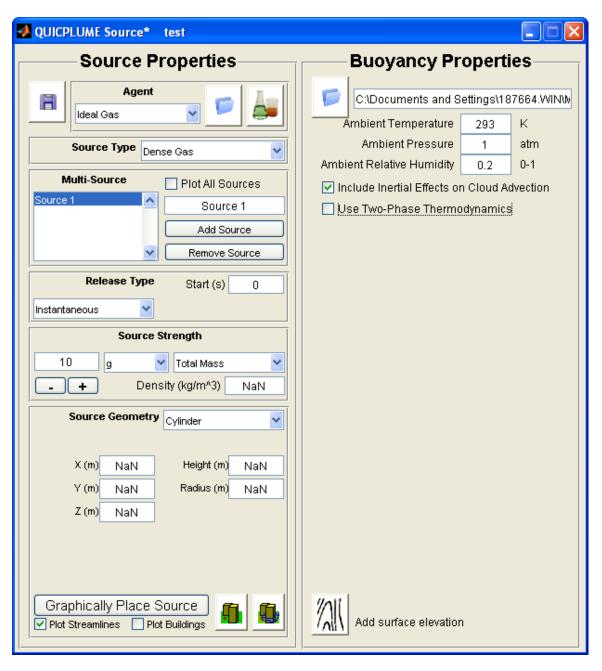

Source Type

The user can pick from eight different source types. They are shown below

Dense Gas

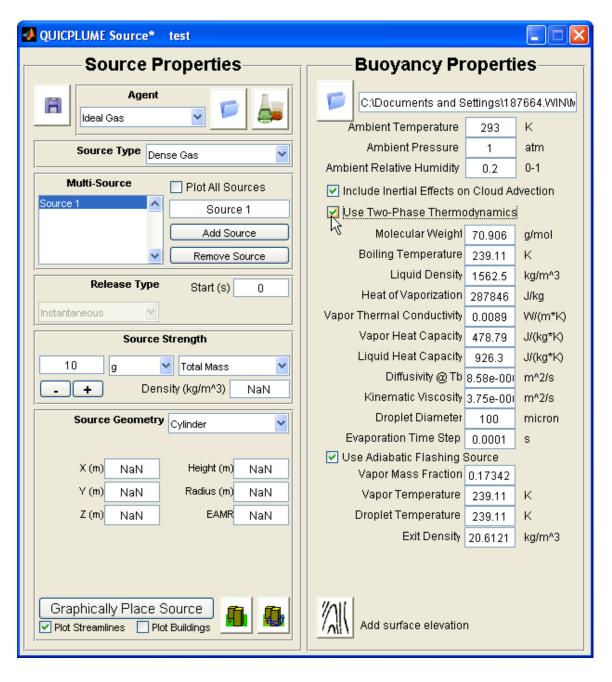Choosing the 'Dense Gas' option brings up the 'Buoyancy Properties' Window.

The user can manually input values for these properties. In order to choose previously saved values, click the open button [icon]. The user is directed to the material library folder or can navigate to the desired QP_buoy.inp file. After choosing the desired QP_buoy.inp file, click on the open button [Open]. This will load these values into the 'Buoyancy Properties' window.

There are two options for dense gas algorithms: 1) the standard slab algorithm which only accounts for entrainment to reduce the density of the cloud and 2) two-phase thermodynamics which accounts for the effects of evaporating droplets on the dense gas dispersion. The standard algorithm can simulate both instantaneous and continuous releases but the two-phase algorithm can currently only be used for instantaneous releases.

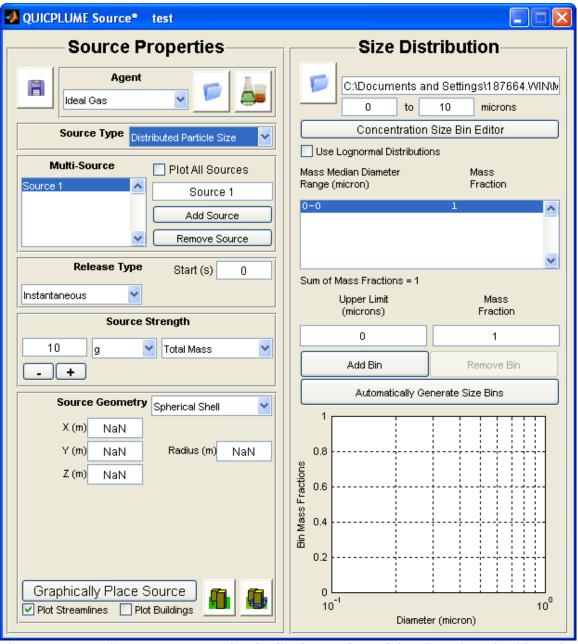If two-phase thermodynamics have been selected then several more parameters become visible.

Most of these parameters can be easily found for a wide range of materials by a simple web search. The diffusivity of the agent at its boiling point is usually the most difficult to find. Often this parameter must be calculated using one of various diffusion coefficient algorithms.

Depending on the agent and the circumstances in which it was released, the release may be assumed to flash adiabatically. When the adiabatic flashing source is selected the vapor mass fraction is determined by a simple balance of the enthalpy released to bring the liquid droplet temperature down to the boiling temperature and the latent heat of vaporization. This assumes that the agent is stored at some temperature above the boiling point at a pressure sufficiently large to condense the agent in the storage tank. When the agent is released from the tank it is released as liquid droplets of the specified size. Part of these droplets evaporate almost instantly (flash) due to the sudden change in pressure upon being released into the atmosphere. This evaporation takes place so quickly that it can be assumed to only occur within the droplet. The mass that is evaporated from the droplet takes the energy it needs to change phase from the enthalpy of the remaining liquid in the droplet.

Distributed Particle Size

Choosing the 'Distributed Particle Size' option brings up the 'Particle Size Distribution' window as shown below.

The user can choose 'Lognormal Distribution' of particle sizes by checking the 'Lognormal Distribution' check box.
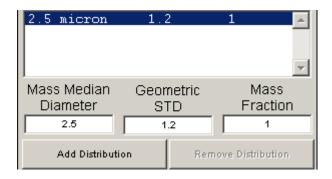
The log normal distributions can be distributed by either mass or by particle count. The distribution type is selected with the pop-up menu next to the checkbox that enables the log normal distribution option.
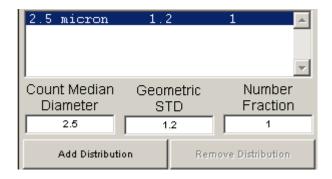

Log normal distributions are defined by a representative diameter (μ), which is the mass median diameter in the case of distributions by mass and count median diameter in the case of distributions by count, and a geometric standard deviation (σ). These parameters define a probability density as a function particle diameter (d) shown below:

$$pdf = \frac{1}{d\sigma\sqrt{2\pi}} \exp\left(0.5\left[\frac{\ln(d) - \ln(\mu)}{\ln(\sigma)}\right]^2\right)$$
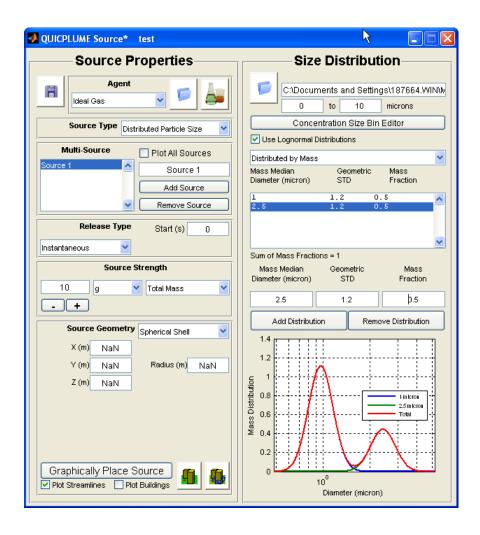
In the case where multiple distributions are used to define the total distribution a mass fraction (for mass distributions) or a number fraction (for count distributions) is also required. If the user chooses the 'Distributed by Mass' option, he / she can enter the values of the mass median diameter, geometric standard deviation and mass fraction in the input box as shown below.

If the user chooses the 'Distributed by Number' option, he / she can enter the values of the count median diameter, geometric standard deviation and number fraction in the input box as shown below.

The user can add distributed particle sizes by clicking the 'Add Distribution' button and entering the values of the mass median diameter, geometric standard deviations etc of the various particle sizes. This is shown below.

To remove any distributions, the user can select the distribution with the cursor and click on the 'Remove Distribution' button
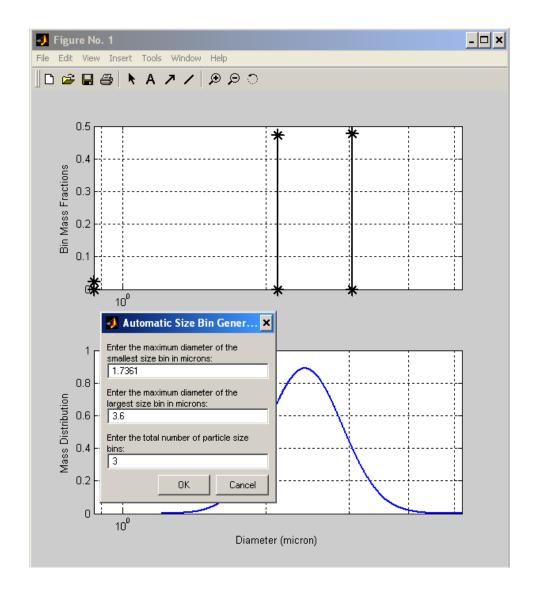
.

If lognormal particle size distributions option is not selected, QUICPLUME can use a particle size distribution composed of discrete bins with corresponding mass fractions. In case of multiple particle size bins, the lower limit of the second bin (bin with bigger particle sizes) is taken as the upper limit of the first bin (bin with smaller particle sizes). QUICPLUME assumes that all of the particles in a particular bin have the mean bin diameter. The smallest bin has a lower limit of zero yielding a mean size of half the upper limit.

Mean Size of particles in a bin = (Upper Limit + Lower Limit) / 2

For example, if there were two bins with particle sizes distributed between 0-5 micron and 5-10 micron; the mean particle size for the first bin would be (0+5) / 2 = 2.5 micron; the mean particle size for the second bin would be (5+10)/2 = 7.5 micron (upper limit of first bin = lower limit of the second bin).

The 'Particle Size Distribution' window provides the user the option of either entering these bins manually using the 'Add Bin' button [Add Bin] or they can use the 'Automatically Generate Size Bins' option [Automatically Generate Size Bins] to produce discrete size bins from the lognormal distributions.

Note: This function was originally introduced when the discrete size bins were the only method to input particle size distributions. Now that QUIC-PLUME uses the lognormal distributions to produce continuous particle size distributions directly, this functionality is obsolete.

In the 'Automatic Size Bin Generator' window, enter the values as shown and press the 'ok' button [OK]. This leaves the user with a figure showing the 'Bin Mass Fraction' and 'Mass Distribution' with respect to the bin diameter.
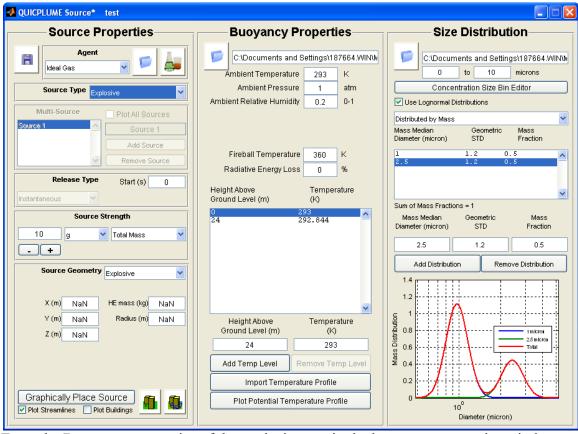
Closing this figure takes the user back to the main 'Particle Size Distribution' window and here the user can see the bins generated and their corresponding mass fractions.

In order to choose previously saved particle distributions, click the open button [📂]. The user is directed to the material library from where he / she can choose a previously saved QP_particlesize.inp file or the user may navigate to a previously saved project and load the QP_particlesize.inp file from another project folder. After choosing the desired file, click on the open button [Open]. This will load the new values into the 'Particle Size Distribution' window.

Explosive

Choosing the 'Explosive' option brings up the 'Buoyancy Properties' and 'Particle Size Distribution' window as shown below. Using this option QUIC-PLUME computes the buoyant rise of the plume internally using the initial explosion characteristics and the thermal properties of the atmosphere entered in the Buoyancy Properties panel. This source type is recommended over the ERAD source type, which also simulates explosive releases, because this method takes into account the effects of the local winds on the buoyant plume.

Enter the Buoyancy properties of the explosive gas in the buoyancy properties window.

Temperature levels can entered manually by typing in the values in the 'Height Above Ground Level' and 'Temperature' boxes and clicking the 'Add Temperature' button

Existing temperature profiles (if any) can be imported using the 'Import Temperature Profile' button [Import Temperature Profile]

The potential temperature profile (measured from ground level with the adiabatic lapse rate) can be visualized by pressing the "Plot Potential Temperature Profile" button [Plot Potential Temperature Profile]
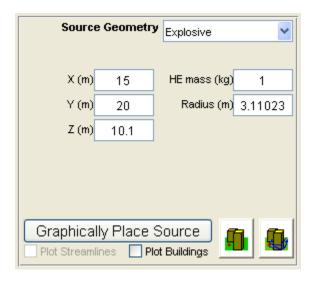
Enter the values in the 'Particle Size Distribution' window based on the explanation given in the previous section.

After performing these steps, move to the 'Source geometry' portion of the main window. Here the user will find the source geometry as 'Explosive'.
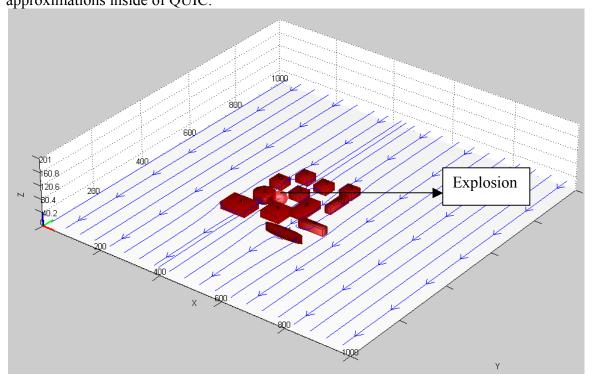
Enter the locations and mass of the high explosive (HE) in kg. The initial blast radius (one atmosphere overpressure radius) and approximate height of the plume after it comes to equilibrium are calculated based on the amount of HE mass. This is shown below.

To view the location of the explosive in the city, the user can use the 'View source placement in the city' button .

The latest version of the explosive source calculates building damage radii and may require QUIC-URB to be run again. The first radius at 15 psi overpressure destroys all buildings within it and makes these buildings inactive (which is why QUIC-URB must be run again if it has already been run). The second radius at 1 psi overpressure damages the buildings (i.e., makes them much more leaky for purposes of building infiltration calculations discussed in a later section). This building damage model is obviously
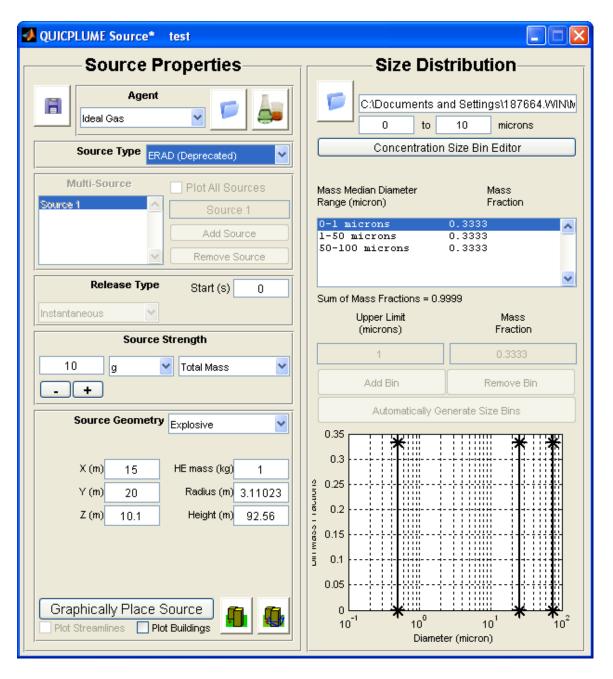
highly simplified from reality but is likely sufficient given all of the inherent errors and approximations inside of QUIC.

ERAD

Choosing the 'ERAD' option brings up the 'Particle Size Distribution' window as shown below. The ERAD source type also simulates an explosive release similar to the Explosive source type. The principal difference lies in the fact that for this source the particle distributions and equilibrium plume are initialized at the source location using output from the ERAD model. Thus, it is assumed that the time that it takes for the buoyant plume to come to equilibrium is negligible and the distribution of the various sizes of particles in the plume occurs instantaneously.
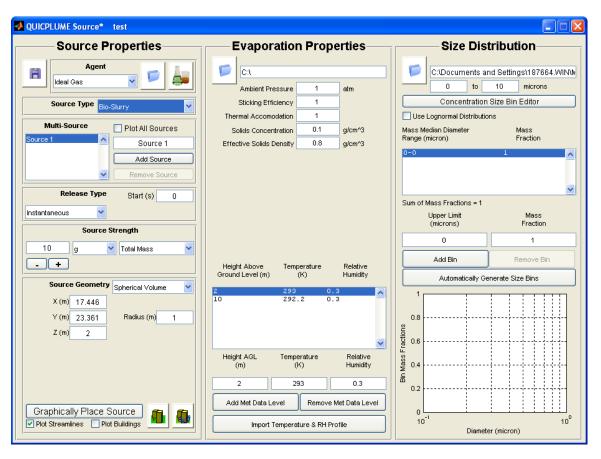
The user can import previously saved parameters by clicking the 'open' button ____ and navigating to the desired QP_erad.inp file from the material library folder or he / she can use any other files by navigating to their respective folders.

Under the 'Source Geometry' section, enter the location and mass in kilograms. To view its location in the city, the user can use the 'View source placement in the city' button
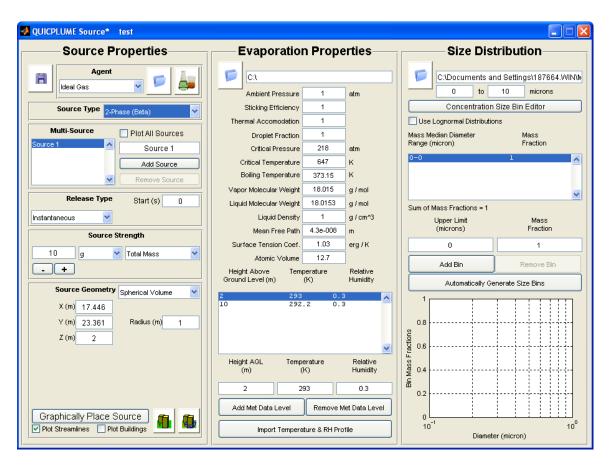
.

Bio-Slurry

Choosing the 'Bio-Slurry' option brings up both the 'Evaporation Properties' and 'Size Distribution' panels. The bio-slurry source type simulates a source that is a mixture of water and a biological agent. Once the mixture is aerosolized the water will evaporate off of the droplets depending on the temperature and relative humidity of the air. The size distribution defines the initial sizes of the droplets. The 'solids concentration' and 'effective solids density' are used to determine the minimum size that the droplets will become after all of the water is evaporated off. 'Solids concentration' refers to the mass of solids within each mL of solution. 'Effective solids density' takes into account the fact that the solids will still have gaps between the particulate after all of the water has evaporated off. The bio-slurry algorithm assumes that all of the solids stay together, i.e., will not break apart further after all of the water is gone.

Two-Phase

The two-phase source type uses the same evaporation algorithm as the bio-slurry source type but instead of assuming the evaporation properties of water it uses several additional algorithms to estimate some of the physical properties of the agent. When the '2-Phase' option is selected both the 'Evaporation Properties' and 'Size Distribution' panels become visible but there are quite a few more parameters in the 'Evaporation Properties' panel which must be defined.
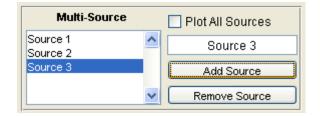
Multi-Source

Some source types (basic and distributed particle size) can have multiple sources in a single simulation. The user can choose multiple sources by clicking on the 'Add Source' [Add Source] button under 'Multi-Source'

For each of the sources added, the user can input different source parameters by selecting the source and entering the values of the various parameters

To remove a source, the user can select the source with the cursor and click on the 'Remove Source' button [Remove Source]
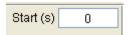
By default only one source is shown in the Plume Source Placement window at a time. Checking the Plot All Sources checkbox causes all of the sources to be plotted at the same time.

Release Type

Three different release types can be selected from the pull-down menu: instantaneous, continuous, and finite duration as shown below. 'Instantaneous' means that all of the particles are released at once. 'Continuous' means that the particles are released at a constant rate from the source start time through the entire duration of the simulation. 'Finite Duration' means that the particles are released at a constant rate for the amount of time entered in the text box that appears next to the release type pull-down menu when finite duration is selected.

The user can specify the start time for the release by entering the time in the 'Start (s)' window as shown below. The default value for the 'instantaneous' and 'Continuous' type releases is set to zero. This is feature is primarily intended for multiple sources which do not start at the same time.
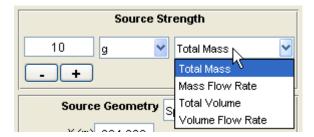

For the 'Finite Duration' type release, the user should specify the start time and duration of the release as shown below.
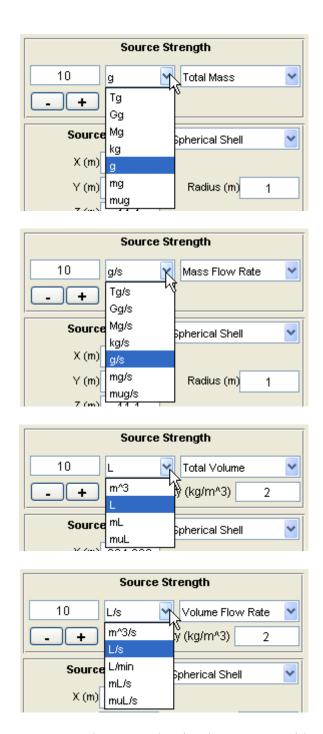

Source Strength

The size of the release is controlled through the "Source Strength" text box. The amount released can be represented as total mass, mass flow rate, total volume and volume flow rate as shown below.
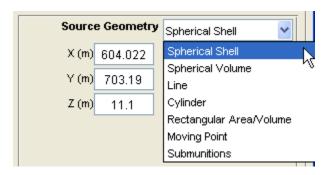
Choosing the source strength type determines the units available in the Source Strength Units Pull-Down Menu as is shown below. Since QUIC-PLUME always uses mass for material amounts, volumetric source types also require a fluid density in kg/m^3.

After selecting the source strength type and units the user can either use the edit box to edit the source strength value or increase or decrease the value using the increment – decrement buttons

Source Geometry and Placement

Six source geometries are available to the user in QUIC-PLUME. They are sphere, line, cylindrical area & volume, rectangular area & volume, explosive, moving point sources, and submunitions sources. The source type selected determines the geometries that are available for use in a project. Currently the dense gas source is uses the cylindrical area/volume source and the explosive source geometry is only used in the explosive and ERAD source types. The geometries that are available for basic and distributed particle size source types are shown in the figure below.
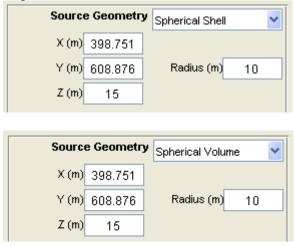
Choosing 'Spherical Shell' or 'Spherical Volume' creates a sphere centered at the location specified in the X, Y, Z location text boxes with the given sphere radius. The shell places all of the particles at the radius specified while the volume distributes the particles evenly throughout the sphere. 'Line' creates a straight line between the points defined in the X, Y, Z begin and end point text boxes. Note that the line can have multiple segments, choosing the segment updates the beginning and end point edit boxes with the values for the selected line segment. Choosing 'Cylinder' creates a cylinder centered at the location specified in the X, Y text boxes with the given height and radius. Note that choosing a height of zero creates a circular area source. Choosing 'Rectangular area / volume' creates a volume with the specified length, width and height. Note that choosing one of the dimensions as zero can result in a 2D plane area source. Choosing 'Moving Point' allows one to create a path between user-specified waypoints and to specify a velocity of the point at each way point. The source will have a constant acceleration between way points determined by the beginning and ending velocities. Particles are randomly placed on a line, along the traveled path over a time step, in a plane, or within volumes when released.

The source location can be set using the text boxes or by clicking 'Graphically Place Source'. Notice that as you graphically move the source around, the X and Y locations update automatically and the z location adjusts if the source is dragged over a building.
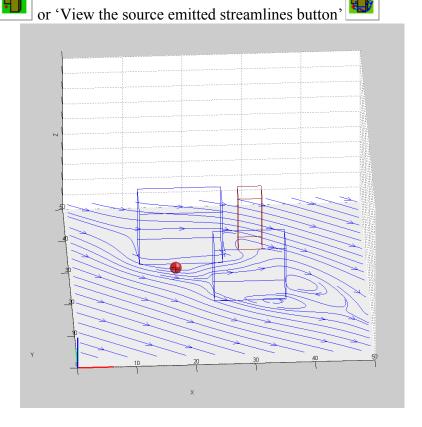
Spherical Shell and Volume

To place a spherical source where all of the particles are placed at the radius, select the source geometry as 'spherical shell' and enter the co-ordinates of the location and radius of the sphere as shown below. Selecting 'spherical volume' evenly distributes the particles throughout the spherical volume.
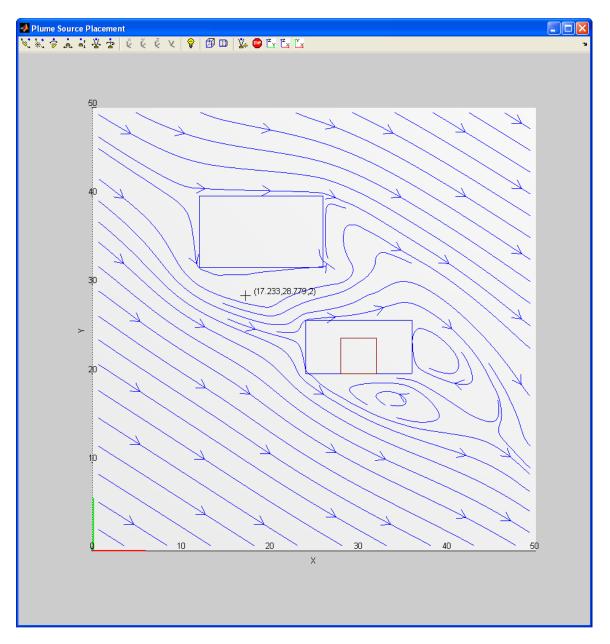

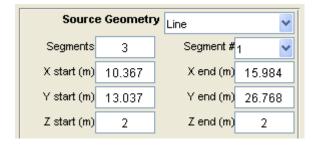To view the location of the source, press either the 'View the source placement within the city' button or 'View the source emitted streamlines button'

To graphically place the source, click the 'graphically Place Source' button
Graphically Place Source
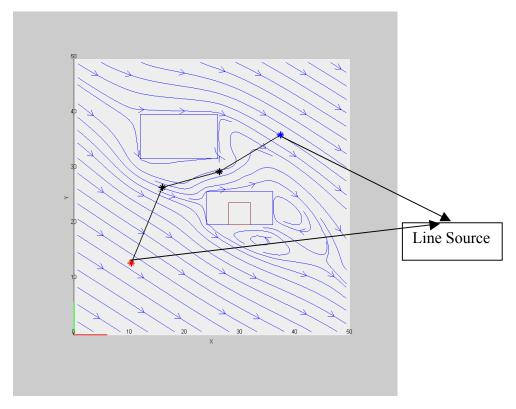
This will launch a 'Plume Source Placement' window shown below. With the cursor, place the source at the desired location. The 3D image manipulation buttons at the top of the window can be used to zoom in on a particular area of the city if greater detail is required for graphical source placement.

Line

To place a line source using the text box option, select the source geometry as 'line' and enter the co-ordinates of the start and end locations of the line as shown below. Alternatively, this could be done using the 'Graphically Place Source' option. Graphically defining a line source involves left-clicking the number of segments plus one locations on the Plume Source Placement window to define the beginning and end of all the segments.
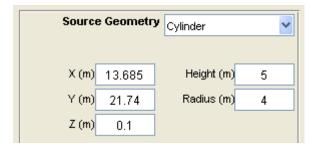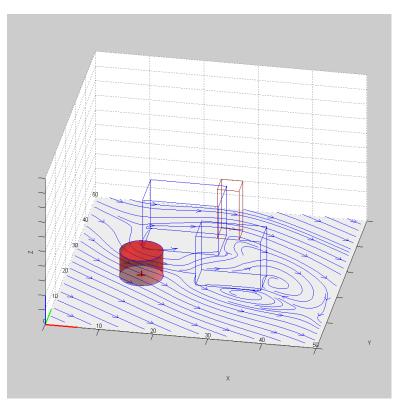
Cylindrical Area/Volume

To place a cylindrical source using the text box option, select the source geometry as 'cylinder' and enter the co-ordinates of the location of the cylinder and also the height and radius of the cylinder. Alternatively, this could be done using the 'Graphically Place Source' option.
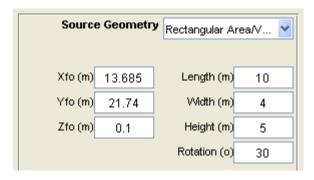
Note: This is the only source geometry available for dense gas source types.
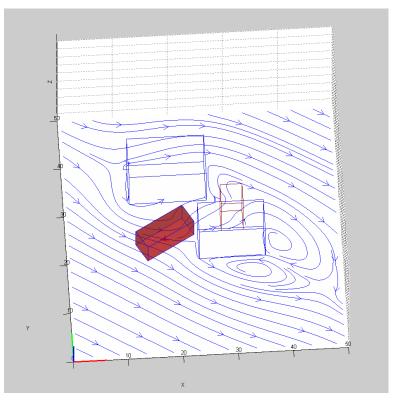
Rectangular Area / Volume

To place a rectangular source using the text box option, select the source geometry as 'Rectangular Area / Volume' and enter the co-ordinates of the location of the source and also length, breadth and height (if the source is a volume). Alternatively, this could be done using the 'Graphically Place Source' option.
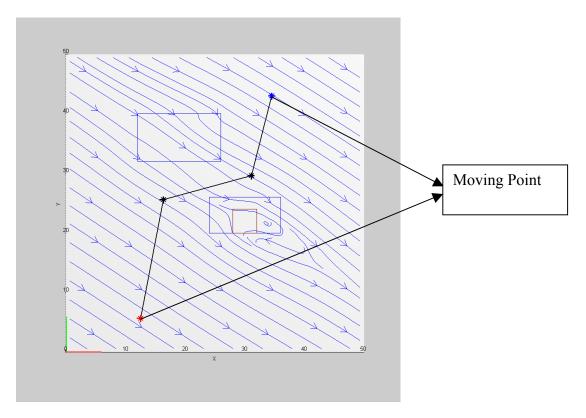
Moving Point

To place a moving point source using the text box option, select the source geometry as 'Moving Point' and enter the co-ordinates of the start and end locations of the source and also velocity of the source at the start and end locations. Alternatively, this could be done using the 'Graphically Place Source' option.
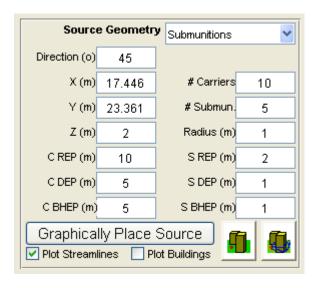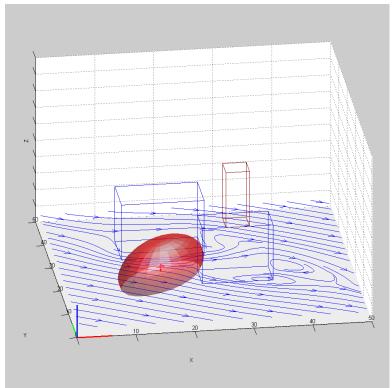

Note: There are checks in the graphical source placement functions to prevent the placement of any part of the source inside of a building and the vertical position of the source is automatically selected to avoid placing any part of the source inside of a building.

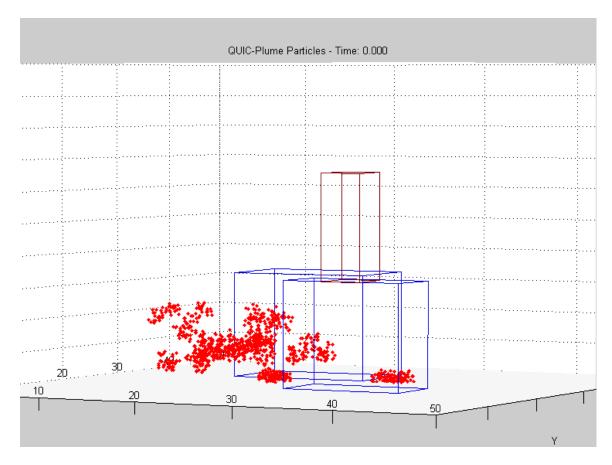You will need to click on to save current parameters and close the Source Placement Window.

Submunitions

The submunitions source geometry is intended to simulate a source generated from multiple carriers (projectiles) launched at a target. Each of these carriers can break apart into a user specified number of submunitions (smaller projectiles) before impact. Due to the probabilistic nature of this type of source, it is defined by the target location, the direction of fire, and the range, deflection, and burst height error probable for both the carriers and the submunitions. It also uses the number of carriers and number of submunitions per carrier.
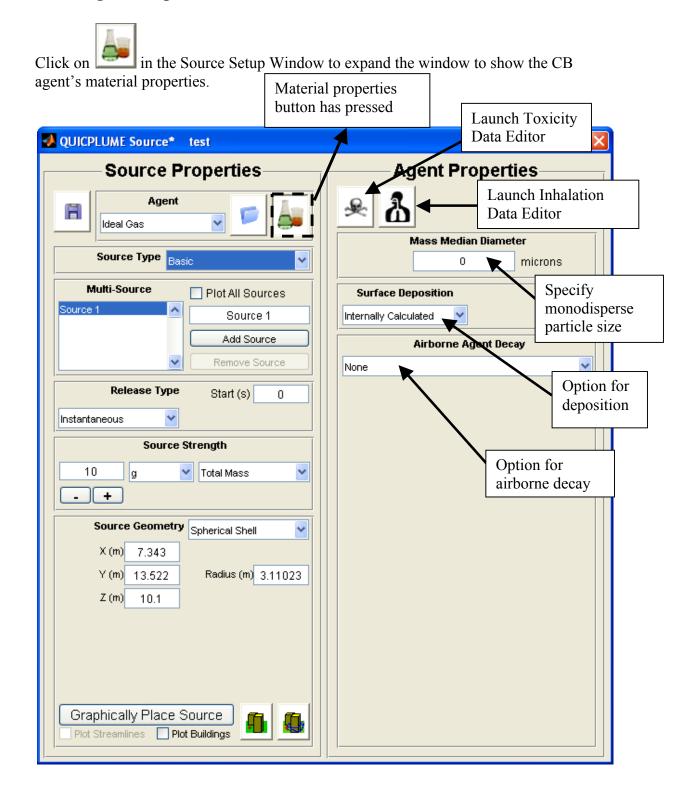
Inside of QUIC-PLUME the final location of each submunition are distributed using the error probable values. The figure below shows the actual initial particle positions produced using the submunitions source geometry shown above. Note the spotty nature of this source type.
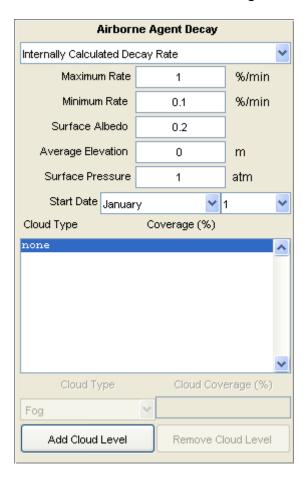

QUIC-Plume Particles - Time: 0.000

Basic Agent Properties

Click on [flask icon] in the Source Setup Window to expand the window to show the CB agent's material properties.

Particle Size

For the basic source type a single particle size can be specified. A value of "0" indicates a vapor. Multiple particle sizes can be specified for some source types. For these source types the process for defining the particle size distribution is detailed in "Distributed Particle Size" source type section.

Surface Deposition

Surface deposition can be specified in one of two ways: a user specified constant deposition velocity or internally calculated based on particle size dependent settling velocity. It is recommended that a constant deposition velocity be used for vapors while internal calculation be used for sources with a particle size.

Airborne Agent Decay

Airborne agent decay can either be a user specified constant decay rate or an internally calculated decay rate based on the UV insolation. The user specifies the minimum (with no insolation) and maximum (mid day insolation) decay rates for the agent, the surface albedo, average elevation of the domain, surface pressure, day of the year, and the number and types of clouds as well as the amount of coverage for each layer.

The following cloud types are available and they are arranged in order of the altitude at which they are typically found.
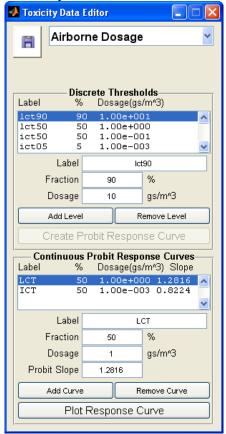

Up to 9 cloud layers can be defined and cloud types can be duplicated (e.g., two layers of stratus and 3 layers of cumulus, etc.). The cloud layers act to attenuate the insolation at the surface.
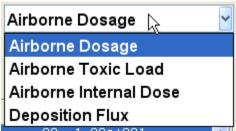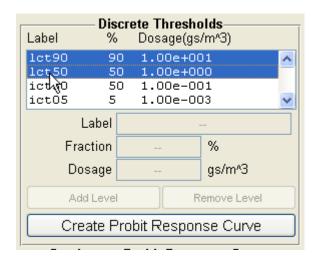
Toxicity Data Editor

Click on to launch the toxicity data editor.

In the toxicity data editor both discrete thresholds and continuous probit slope dose response curves can be defined for airborne dosage, airborne toxic load ($=(gm^{-3})^n s$, where n is the toxic load exponent), airborne internal dose (defaults to grams but the user can specify custom units such as spores for some biological agents), and deposition flux (). Most toxicity data can be entered after QUIC-PLUME has been run as a post processing step. The notable exception to this is the toxic load exponent which must be specified before running QUIC-PLUME and will require QUIC-PLUME to be rerun if it is modified. This is due to the non-linear nature of the toxic load equation.
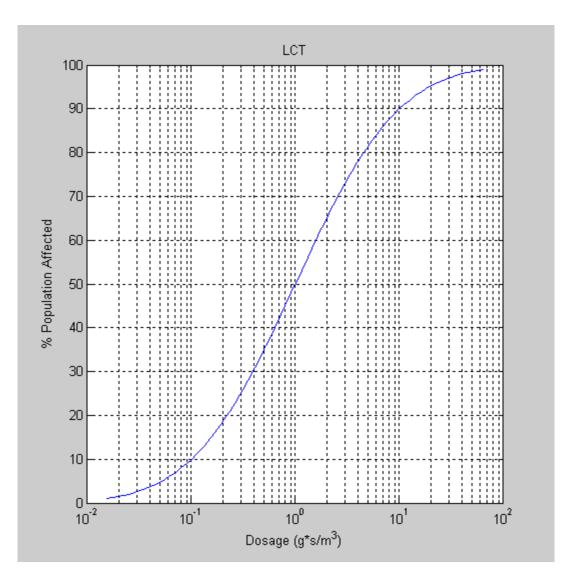

A probit slope dose response curve can be created automatically from two discrete thresholds. Simply hold the <control> or <command> key (depending on platform) to select multiple discrete thresholds from the list as is seen below:

This will cause the [Create Probit Response Curve] button to become active. Press this button to automatically create a new probit response curve which will be added to the list of continuous probit response curves for the selected exposure type.

Pressing the [Plot Response Curve] button produces the following plot.

Airborne Dosage

Airborne dosage is defined as time integrated concentration, where concentration is the mass of the agent per unit volume. This is appropriate when only the total amount of exposure is important, i.e., exposure to a high concentration over a short period of time and an exposure to a low concentration over a long period of time have the same toxic effect. QUIC uses dosage units of gsm^{-3}.

$$D = \int Cdt$$

Airborne Toxic Load

Toxic load is similar to dosage, but there is an exponent power on concentration. This is to take into account that for some agents (typically chemicals) can be metabolized by the body to some extent so exposures to low concentrations over a long period of time are not as toxic as exposures to high concentrations over short periods of time. This means that the units of toxic load are somewhat unusual, i.e., $(gm^{-3})^n s$.
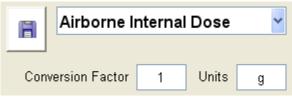
$$T = \int C^n dt$$

When toxic load is selected in the exposure type popup menu, the toxic load exponent edit box appears. The default value for the toxic load exponent is "1". This makes toxic load equivalent to dosage. A value that does not equal "1" informs QUIC-PLUME that it needs to produce the toxic load arrays, which are not written out by default.

Airborne Internal Dose

Airborne internal dose is used with the inhalation model. It takes calculates the actual amount of agent deposited in the various regions of the respiratory tract and uses several parameters about the type of breathing (oronasal or nasal), breathing rate, and the deposition efficiency in the various regions of the respiratory tract. The default units are simply a mass in grams deposited, however, the user can specify custom units (e.g., spores for some biological agents) with a conversion factor between grams and the custom units. When internal dose is selected the conversion factor and custom units edit boxes appear.
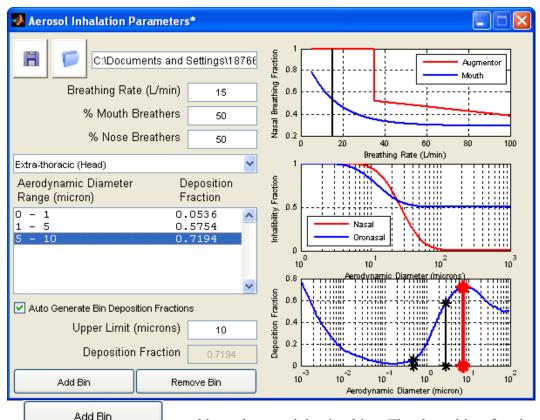

grams*Factor = user specified units

Surface Deposition Flux

Some agents are not only toxic in their airborne forms but also through cutaneous (contact with skin) exposure. For these agents the surface deposition flux toxicity data is also of interest. Surface deposition flux has the units of gm^{-2}.

Aerosol Inhalation Parameters

Most of the aerosol inhalation parameters can be modified as a post processing step. While the particle size distribution can be defined by continuous log-normal distributions the inhalation model itself uses discrete bins. The particle size bins used to calculate the size dependent dosage which is in turn used to calculate the internal dose. These calculations are performed inside of QUIC-PLUME and must therefore be defined before QUIC-PLUME is run. The internal dose that an individual receives is dependent on the breathing rate and the mode of breathing that the individual uses: mouth or augmentor. The percentages of the two breather types is used in population exposure calculations. The data used in the inhalation model were taken from McClellan et al. 2007. Mouth breathers always use both their nose and mouth to breath but the ratio is dependent on breathing rate. Augmentors only breathe through their nose up to a breathing rate of 35 L/min, after which they use both the nose and mouth with a ratio that is breathing rate dependent (see plot on upper right of the figure below). The middle plot shows the inhalability of aerosols as a function of particle diameter. The lower plot is the deposition efficiency as a function of particle diameter for the region of the respiratory tract selected in the popup menu on the left. The blue line in the bottom plot represents the continuous deposition data from McClellan et al. 2007. QUIC-PLUME tracks size dependent airborne dosage in discrete bins. In practice, all of the particles in a bin are treated as if they had the mean diameter of the bin, which is represented by the red and black vertical lines in the bottom plot. The currently selected bin is highlighted in red. This plot is intended to indicate how well the user-defined bins represent the continuous curve over the range in particle diameters of interest.

Press ![Add Bin] to add another particle size bin. The deposition fraction of the bin can either be determined automatically from the continuous data by selecting the auto generation check box. If the check box is not selected then the deposition fraction edit box is enabled.

Agent Library

One can define the following agent properties: decay rate, mass median diameter, deposition velocity, toxic load exponent, discrete thresholds and continuous probit slopes for airborne dosage, airborne toxic load, inhaled internal dose, and surface deposition flux. Default values appear based on the agent type selected in the Agent Type pull-down menu to the left. These values are found in a text file called *default_materials.lib* found in the *material_library* subdirectory. The public release version contains a library file with generic agents (ideal gas, 5 micron particles, etc.) that have artificial material property values. An unclassified official use only agent library is provided upon request to government and other qualified users.

New agents can be added to the library. Simply append the new agent's material properties to the end of the *default_materials.lib* file in the *material_library* subdirectory. The format for the material agent entries is comma delimited in the following order:
1. Material name
2. Decay rate (%/min)
3. Mean particle diameter (micron)

4. Deposition velocity (cm/s)[a value of -99 indicates internally calculated deposition velocity and a value of 0 indicates no deposition]
5. Number of airborne dosage probit slope response curves
6. The airborne dosage probit slope data (if any):
    a. first probit label string, population percentage, dosage (g*s/m^3), and slope
    b. second probit label string , population percentage, dosage (g*s/m^3), and slope
    c. etc.
7. Number of discrete airborne dosage thresholds
8. The airborne dosage discrete threshold data (if any):
    a. first discrete threshold level value (g*s/m^3) and label string
    b. first discrete threshold level value (g*s/m^3) and label string
    c. etc.
9. Toxic load exponent (n)
10. Number of airborne toxic load probit slope response curves
11. The airborne toxic load probit slope data (if any):
    a. first probit label string, population percentage, toxic load (s*[g/m^3]^n), and slope
    b. second probit label string , population percentage, toxic load (s*[g/m^3]^n), and slope
    c. etc.
12. Number of discrete airborne toxic load thresholds
13. The airborne toxic load discrete threshold data (if any):
    a. first discrete threshold level value (s*[g/m^3]^n) and label string
    b. first discrete threshold level value (s*[g/m^3]^n) and label string
    c. etc.
14. Internal dose conversion factor [conversion from grams to the user specified units]
15. Internal dose units label
16. Number of airborne inhaled internal dose probit slope response curves
17. The airborne inhaled internal dose probit slope data (if any):
    a. first probit label string, population percentage, internal dose (user specified units or grams[default]), and slope
    b. second probit label string , population percentage, internal dose (user specified units or grams[default]), and slope
    c. etc.
18. Number of discrete airborne inhaled internal dose thresholds
19. The airborne inhaled internal dose discrete threshold data (if any):
    a. first discrete threshold level value (user specified units or grams[default]) and label string
    b. first discrete threshold level value (user specified units or grams[default]) and label string
    c. etc.
20. Number of surface deposition flux probit slope response curves
21. The surface deposition flux probit slope data (if any):

> a. first probit label string, population percentage, surface deposition flux (g/m^2), and slope
> b. second probit label string , population percentage, surface deposition flux (g/m^2), and slope
> c. etc.

22. Number of discrete surface deposition flux thresholds
23. The surface deposition flux discrete threshold data (if any):
> a. first discrete threshold level value (g/m^2) and label string
> b. first discrete threshold level value (g/m^2) and label string

24. etc.

Ideal Gas,0.,0.,0.,2,LCT,50,1,1.2816,ICT,50,1e-3,0.8224,4,10,90,lct90,1.0,50,lct50, 1.0e-01,50,ict50,1.0e-03,5,ict05,1.0,0,0,0,1.0,g,0,0,0,0,

After making any changes in the Source Parameter Set-up Window, you will need to click on [image] to save current parameters and close the Source Placement Window. Note that this save the modified values in the project but not the actual library, which can only be changed by manually editing the *materials.lib* text file.
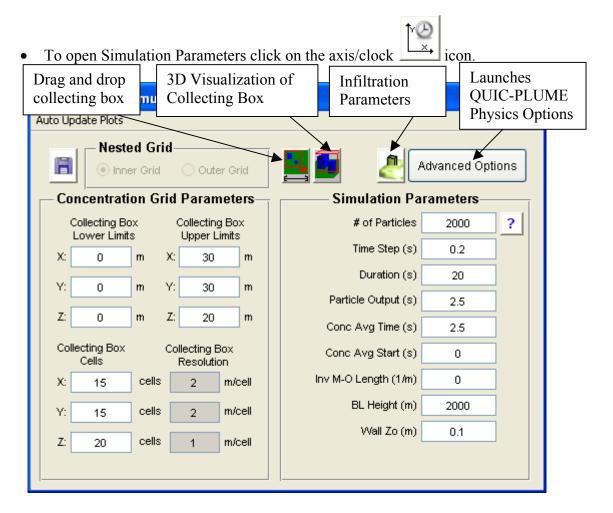
Another agent library can be used instead of the *default_materials.lib* file by pressing the [image] button and navigating to the desired *materials.lib* file. This button is found to the right of the agent selector popup menu.

QUIC-PLUME Simulation Parameters

- To open Simulation Parameters click on the axis/clock [icon]. icon.

Drag and drop collecting box

3D Visualization of Collecting Box

Infiltration Parameters

Launches QUIC-PLUME Physics Options

- The set-up of the concentration domain is done on the left, while several QUIC-PLUME random-walk, averaging time, output frequency, and turbulence model parameters are specified on the right. Advanced options (such as particle splitting, etc.) are defined in the QUIC-PLUME Physics Options GUI which is launched by the 'Advanced Options' button in the upper-right-hand corner.

- The 3D extent of the concentration grid can be set through the "Collecting Box Lower and Upper Limits". By default, the horizontal extent of the domain is the QUIC-URB modeling domain.

- Specification of the number of grid cells through the "Collecting Box Dimensions" text boxes controls the grid size. The grid cell can be any size and does not need to be equivalent to the grid cell size of the QUIC-URB domain.

- There is a tradeoff in changing the number of particles in the random-walk simulation: more particles results in a computed concentration with less uncertainty, but fewer particles results in a faster simulation. The higher

uncertainty produced by fewer particles may be compensated for by larger collecting box grid cells or longer averaging times. Note that whenever applicable, typically for finite duration and continuous releases, the QUIC-GUI will automatically round-off the number of particles that is entered to satisfy the constraint that an integer number of particles must be released at each time step.

- Pressing the number of particles help button [?] will launch the number of particles calculator.

This calculates the maximum number of particles required to allow QUIC-PLUME to resolve airborne dosages down to a target dosage level. The calculation is simply:

$$n = \frac{M\Delta t}{D\,dx\,dy\,dz}$$

Where n is the number of particles, M is total mass released, Δt is the time step, D is the target dosage, and dx, dy, and dz are the size of concentration collecting boxes in the x, y, and z directions. This calculation assumes that there is no particle splitting, agent decay, or surface deposition which will all act to reduce the number of particles required to resolve the plume down to the target dosage level.

- The simulation time step controls the size of the time step used by the random walk model. A larger time step allows the simulation to proceed more quickly, but the time step must be smaller than the Lagrangian time scale to give accurate answers. The code will internally compute time step constraints and change the time step when necessary. However, choosing an "unreasonable" time step, either way too large or way too small, will lead to problems. For outdoor, real-scale building-resolved problems a time step of a few seconds is reasonable. For wind tunnel scale problems, a tenth of a second time step may be required. Note: a simple approximation for the Lagrangian time scale over a flat surface is kz/u_*, where k is the von Karman constant, z is height above ground, and u_* is the friction velocity. Erring on the side of larger time steps is recommended due to the internal checks and automatic time step reduction algorithm.

- The "duration of the simulation" controls how long the dispersion calculation will proceed. If a finite duration release has been selected, the simulation duration must be at least as long as the release duration.

- The particle output frequency determines how often particle location data is written out to a text file (which is then used in the VIS-GUI to visually illustrate the dispersal of the agent). This parameter does not affect the physics of the random-walk model, it only affects how often particle positions are written out to a file for visualization purposes. When running simulations with large numbers of particles, it is strongly recommended to set this to a large number in order to save disk space (and speed up the simulation). When making animations of particle transport and dispersion, it is recommended that a small number of particles (e.g., 500 to 2000) be used along with a small number for the output frequency (e.g., every time step).

- The QUIC-PLUME code produces time-averaged concentrations in a 3D volume defined by the concentration collecting box. The "Concentration Field Averaging Time" specifies the time interval over which particles are counted in the collecting grid boxes.

- The "Concentration Average Start Time" specifies when the concentration averaging will begin. This is effectively a skip time at the beginning of the particle simulation over which the concentration is not computed. By default it is set to 0. This option is in general only used when trying to compare plume parameters (e.g., concentration) with values from controlled experiments typically taken from a continuous sources under steady-state conditions.

- The "Inv M-O Length" is the inverse Monin-Obukhov length scale. This is a measure of atmospheric thermal stability from Monin-Obukhov boundary layer similarity theory. A value of zero (the default value) is indicative of neutral thermal stability where the turbulence is purely mechanically generated. Positive values indicate thermally stable conditions, typically associated with nighttime, where colder and therefore denser air is closer to the ground. Thermally stable conditions dampen the turbulence in the vertical direction because buoyant forces resist vertical motions. Negative values indicate thermally unstable conditions, typically associated with daytime, when the sun heats the ground causing the air near the ground to be warmer and therefore less dense than the air above it. Thermally unstable conditions enhance the vertical turbulence because the buoyant forces act to move the warm air near the ground up and the colder air above down. In reality strong thermal stability can not only enhance the vertical turbulence but actually affect the mean flow generating thermal convective cells where regions of positive and negative mean vertical velocities will exist in the flow field. This is a complicated process that cannot be simulated by QUIC. Inputting a strong negative value for inverse Monin-Obukhov length will only further enhance the turbulence. The figure below is taken from Golder 1972 and

estimates the inverse MO length as a function of surface roughness (z_o) and Pasquill stability class
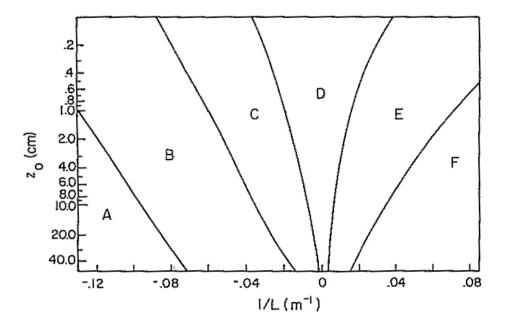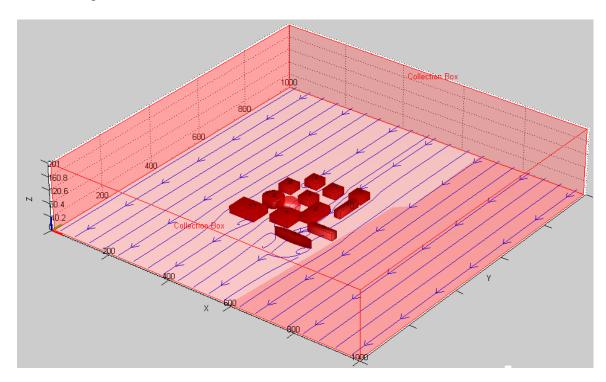
Figure depicts dependence of Pasquill's stability class on surface roughness and inverse Monin-Obukhov length. From Golder, 1972.

- The "BL Height" is the height of the atmospheric boundary layer, i.e., the region of the atmosphere where most directly affected by the surface of the earth. Turbulence in the atmospheric boundary layer tends to diminish with height above the surface. The height of the boundary layer can range from tens of meters under strongly thermally stable conditions to thousands of meters in strongly thermally unstable conditions. Often for small scale problems this effect is not particularly important so the default value of 2,000 meters will not have much of an effect on the turbulence.

- The "Wall Zo" is the aerodynamic roughness length associated with surface of the buildings and ground. The user should be aware that this is not the same thing as the roughness length used in defining the input velocity profile which is intended to capture the bulk effect of the large scale roughness elements (e.g., trees, buildings, cars, etc.) on the area-averaged velocity profile. In this case the wall roughness length is intended for use in interpolations in the velocity field as particles get very close to individual surfaces, and can therefore be expected to have a much smaller value.
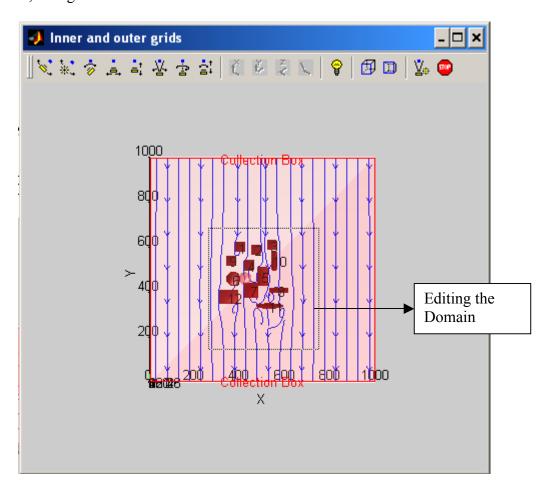
View Current Collecting Box

The 'View Current Collecting Box' ![icon] option helps the user visualize the concentration domain of QUIC-PLUME. This is shown below.

Edit Collecting Box

The 'Edit Collecting Box' provides the user the option of editing the bounds of the

concentration domain. To do this, click on the 'Edit Collecting Box' button and with the cursor, change the limits of the domain. This is shown below.
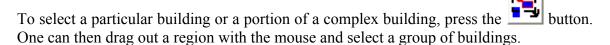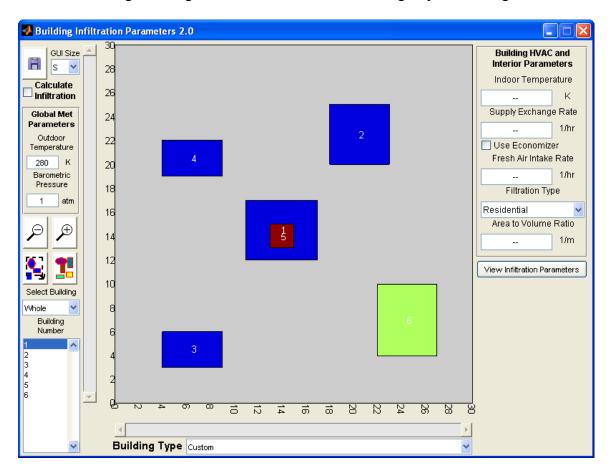
Building Infiltration
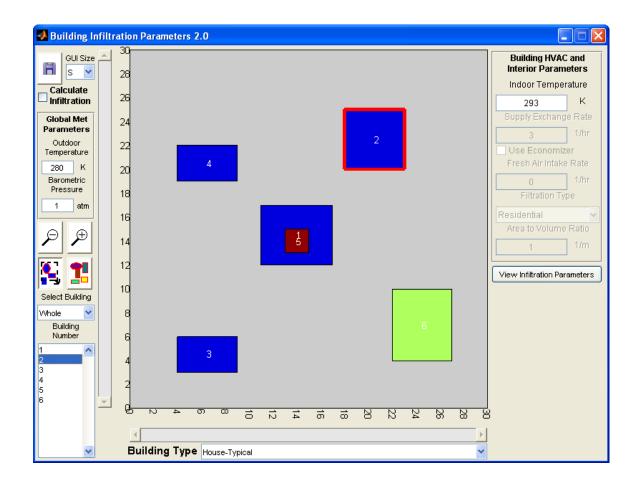
Pressing the 'Building Infiltration Parameters' button opens up a window where the building infiltration parameters can be set. Warning: this is a beta feature and has not been fully tested.

By default, the calculation of building infiltration is turned off in QUIC. In this window, you can turn it on by checking the "Calculate Building Infiltration" checkbox.

To select all the buildings in the domain, press the button.

To select a particular building or a portion of a complex building, press the button. One can then drag out a region with the mouse and select a group of buildings.

Once a building or group of buildings is selected, then the building type popup menu at the bottom of the GUI and HVAC and infiltration parameters on the right-hand side of the GUI are populated with the values for the selected building(s). The infiltration parameters only become visible if the [View Infiltration Parameters] toggle is selected.

One can change the parameters for the selected buildings to the default values from the building infiltration library with the building type popup menu at the bottom of the GUI. If "custom" is selected then the HVAC and infiltration parameters are enabled so that the user can modify the values. Below is a list of the HVAC and infiltration parameters as well as a brief description of each parameter.

- Current Meteorological Parameters:
  - Outdoor temperature - average outdoor temperature throughout the domain during the simulation.
  - Barometric Pressure - average barometric pressure throughout the domain during the simulation.
- HVAC parameters
  - Supply Exchange Rate - the rate at which air travels through the HVAC system and it is the sum of the recirculated air exchange rate and the fresh air intake rate.
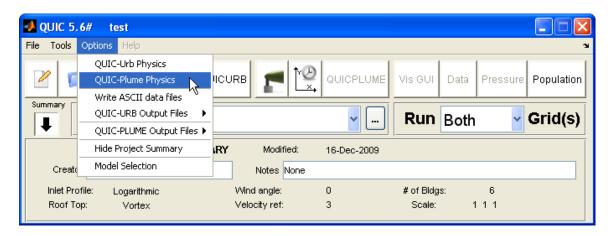
- Use Economizer - HVAC systems with economizers will automatically modify the amount of fresh air intake rate dependent on the outdoor temperature. Outdoor temperatures closer to the standard room temperature will cause the system to have a higher fresh air intake rate.
- Fresh Air Intake Rate - the rate at which the HVAC system brings fresh air from the outside into the building.
- Filtration Type - the class of filtration used for cleaning the aerosol particles out of the air in the building
  - Residential - weakest filtration which filters out primarily only the largest particles. Approximate MERV rating of 4.
  - Commercial - moderate filtration typically found in standard commercial HVAC systems. Approximate MERV rating of 8.
  - Electret - strong filtration typically used in commercial systems where better filtration is required. Approximate MERV rating of 12.
  - HEPA - high-efficiency particulate air filters offer the best protection against aerosol particles. They are typically found in hospitals and clean rooms. Approximate MERV rating of 16.
- Area to Volume Ratio - the ratio of indoor surface area to indoor volume. This includes walls, floors, ceilings, and furniture surfaces. This is used to determine the amount of surface deposition within the building. Note that this does not account for surface orientation so all surfaces indoors will be deposited on evenly.

- Natural Infiltration Parameters - these parameters account for the leakiness of buildings, typically through windows and doors. The parameters are measured at a reference condition and then are modified based on the actual conditions.
  - Indoor Temperature (actual) - The actual indoor temperature at the time of the simulation. Differences in indoor and outdoor temperatures tend to enhance natural infiltration.
  - Infiltration Exchange Rate - the rate at which the building leaks at the reference conditions.
  - Indoor Temperature (reference) - indoor temperature when the reference infiltration exchange rate was measured.
  - Outdoor Temperature (reference) - outdoor temperature when the reference infiltration exchange rate was measured.
  - Atmospheric Pressure (reference) - atmospheric pressure when the reference infiltration exchange rate was measured.
  - Wind Speed (reference) - wind speed when the reference infiltration exchange rate was measured.

The temperature, barometric pressure, and the desired indoor temperature are the current values, the values for the current simulation. QUIC will take these values, along with the wind speed computed by QUIC-URB, and then modify the air exchange rate based on the differences between the reference values and the current values.
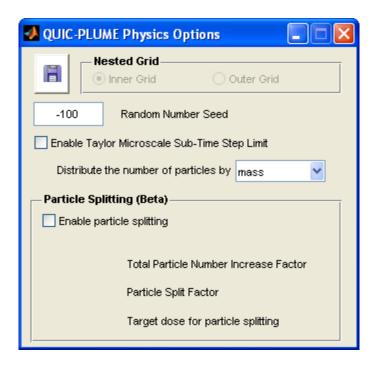
Click on to save current parameters before closing window. This brings the user back to the main QUIC-PLUME Simulation Parameters Window and sends the modified infiltration parameters both to the main QUIC-GUI and the QUIC-PLUME Simulation Parameters Window.

QUIC-PLUME Physics Options

Several parameters used by the QUIC-PLUME dispersion model can be changed through the Physics Options pop-up window. On the main QUIC-GUI window select <Options> <QUIC-PLUME Physics>.

This launches the QUIC-PLUME Physics options GUI as shown below:

Random Number Seed

This changes the random numbers generated by the RAN2 random number generator used to drive the stochastic portion of the random walk model. The random number generation algorithm will always produce identical results for a problem run with the same random number seed. Changing the seed allows the user to change the random numbers that are generated and thus changing the final results (usually only slightly). The changes will be most notable in the tails of the plume which have, by the stochastic nature of the random walk model, the most statistical noise.

Taylor Microscale (Beta)

QUIC-PLUME determines the Lagrangian time scale for each particle and splits the time step into sub-time steps that are at most half of the Lagrangian time scale. The Lagrangian time scale approaches zero as the particle approaches a surface. The Taylor microscale option puts a lower limit on the size of the sub-time steps. This option is experimental and is turned off by default.
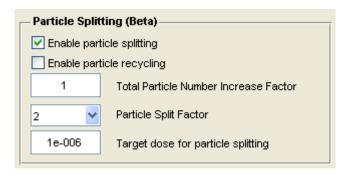
Number of Particles Distribution Method

By default QUIC-PLUME distributes the particles by mass, i.e., the number of particles released by a source in a multiple source problem will be proportional to the amount of mass released by that source. The other option is to distribute the number of particles evenly amongst all of the sources.

Particle Splitting (Beta)

If particle splitting is enabled the particles are split when they enter an empty concentration collecting box. Four parameters are needed when using the particle splitting option:

1. Particle Recycling - This allows the memory used by particles that have left the domain to be used again to split more particles. This is particularly useful for continuous releases with particle splitting.
2. Total particle increase factor - this factor is the multiple of the total number of particles indicated in QUIC-PLUME Simulation Parameters GUI to determine the total number of particles allowed in a simulation. Particles will be allowed to split until the total number of particles reaches this number times the original number of particles in the simulation.
3. Particle split factor - this determines the number of particles a particle will split into when it meets the conditions of splitting.
4. Target dosage - this determines the threshold for particle splitting. Particles will not be split beyond the amount that they can produce this dosage.

Running QUIC-PLUME

Once the QUIC-PLUME source and simulation parameters have been defined and saved, the QUIC-PLUME code can be run (if the parameters are not specified, the QUIC-PLUME button will be deactivated).

- Select the "QUICPLUME" icon.

The light bulb indicates that QUIC-PLUME is running and the wind fields are being computed.
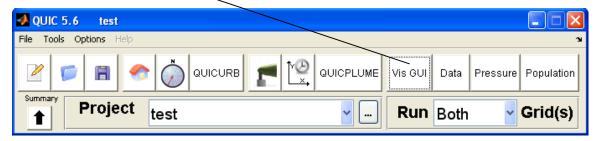
When the light bulb disappears, the model simulation is finished. The output of particle and concentration fields can then be visualized with the Vis-GUI (see next section).

VIS GUI
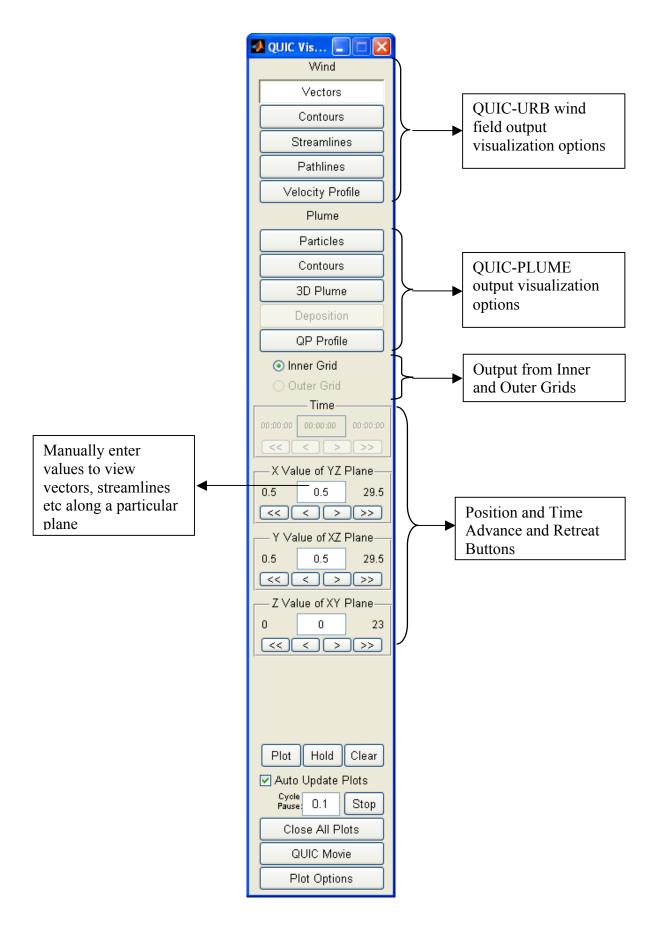
QUIC Visualization GUI

- The Vis GUI first becomes activated once QUIC-URB has been run.

- Press [Vis GUI] to open up the QUIC Visualization GUI as shown below.

- The Visualization GUI opens and it defaults to the wind vector plot selection shown below.

- The QUIC-URB wind field output can be visualized as wind vectors, contours, streamlines, pathlines, and velocity profiles.

- The QUIC-PLUME model output can be visualized as particle positions, contours of airborne quantities, airborne quantity isosurfaces, surface deposition contours, or airborne concentration profiles.

QUIC-URB wind field output visualization options

QUIC-PLUME output visualization options

Output from Inner and Outer Grids

Manually enter values to view vectors, streamlines etc along a particular plane

Position and Time Advance and Retreat Buttons
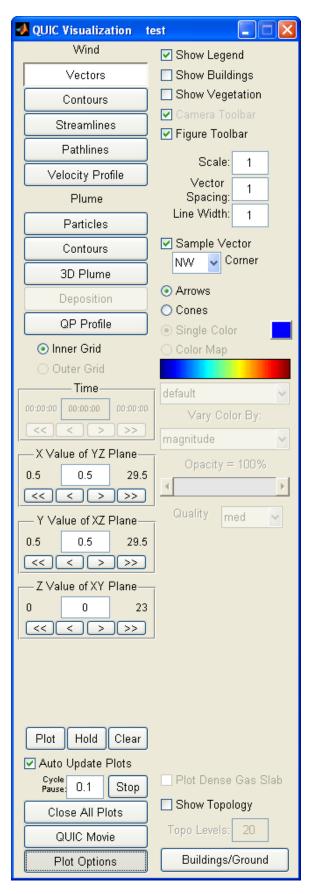
VIS-GUI provides the user a host of options to better view the results. For enhanced effects, press the 'Plot Options' button

at the bottom of the VIS GUI window
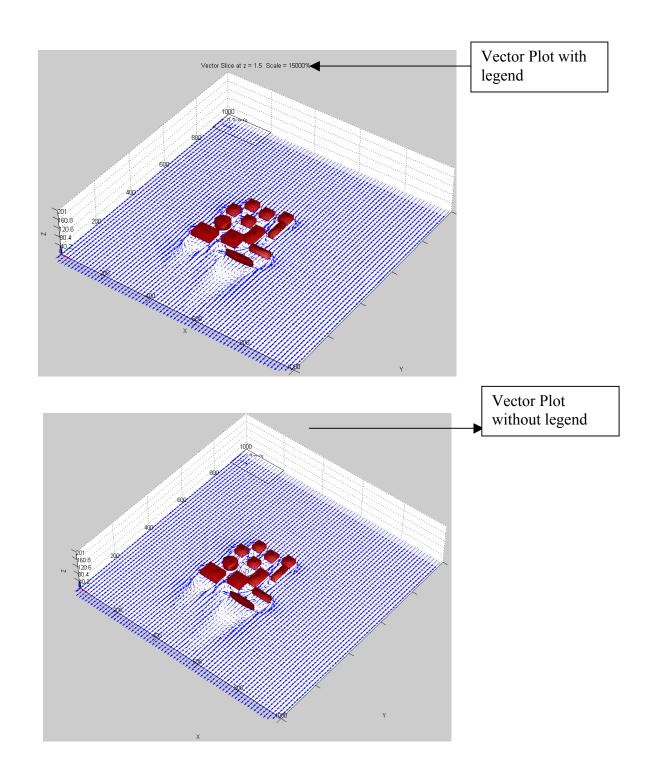
This launches a window with the various plot options as shown to the right. The plot options visible will change depending on which plot type is selected. The options shown are for vector plots. Some of the controls shown are common to several different plot types. This section will start with a description of the general plot controls and will later focus on the plot-type specific controls.
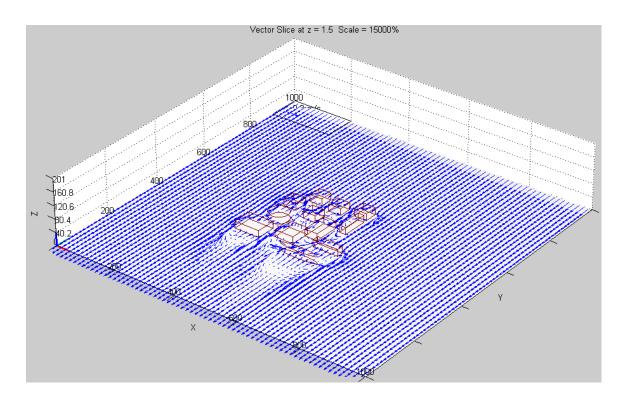
Show Legend

Selecting the 'Show Legend' ☑ Show Legend option places a legend on the vector plot. This also controls if a color bar is shown on the right hand side of the figure.

Vector Plot with legend

Vector Plot without legend
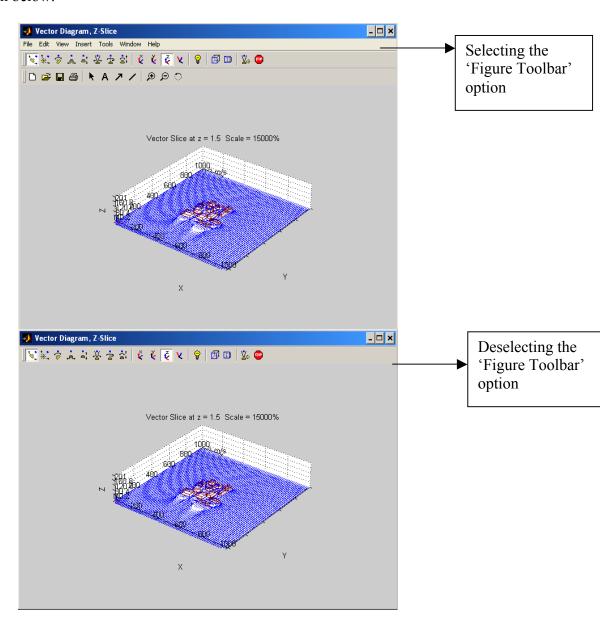
Show Buildings

Selecting the 'Show Buildings' ☐ Show Buildings option displays the buildings in the vector plot. Deselecting it places wire frames instead of buildings. This is shown below

The figure above shows wire frames instead of buildings. This occurs when the 'Show Buildings' option is deselected.

Figure Toolbar

Selecting the 'Figure Toolbar' ☑ Figure Toolbar option displays figure toolbar in the vector plot MATLAB window. Deselecting it does not place it in the MATLAB window. This is shown below.

Selecting the 'Figure Toolbar' option

Deselecting the 'Figure Toolbar' option
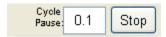
Time and Position Controls

Time and position can be selected by either entering the desired value in the time and position edit boxes or by using the advance and retreat buttons.

The single arrow buttons advance/retreat by a single increment. The double arrow buttons cycle through all possible values from the current time/location to the maximum or minimum value, depending on directionality of the button. The length of time (in seconds) that the GUI pauses in between cycles is set in the 'Cycle Pause' edit box.

The 'Stop' button causes the plots to stop cycling.

Close All Plots
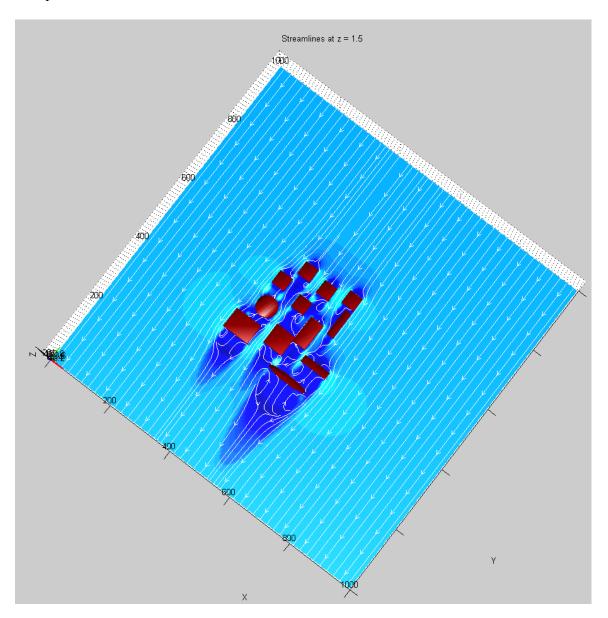
Since each different plot type is generally placed within its own figure window, it is easy to produce several figures in the process of visualizing QUIC data. The 'Close All Plots' button will close all of the figure windows produced by the Visualization GUI. This function is also executed when the Visualization GUI is closed.

Saving Animations

The 'QUIC Movie' button launches the QUIC Movie GUI which produces animations from the plots produced by the Visualization GUI. The details regarding the procedures of movie creation will be discussed later in the QUIC Movie GUI section.

Hold Plot

Multiple plots can be placed on a single figure using the 'Hold' button Hold . After producing a plot pressing the 'Hold' button will hold the current plot and cause future plots to plot to the held figure. Multiple plots can be held on a single figure. Below is an example of the combination of velocity magnitude and streamline plot produced using the hold plot button.

Pressing the 'Clear' button Clear will delete the held figure and will cause the GUI to plot different plot types in different figures.

Buildings / Ground

The Buildings / Ground button [Buildings/Ground] found at the bottom of the VIS GUI window is the same as the one in the City Builder Window. It enables the user change the color of the buildings and the ground; add transparency to both these entities and a host of other options. For these options, please refer the City Builder section.
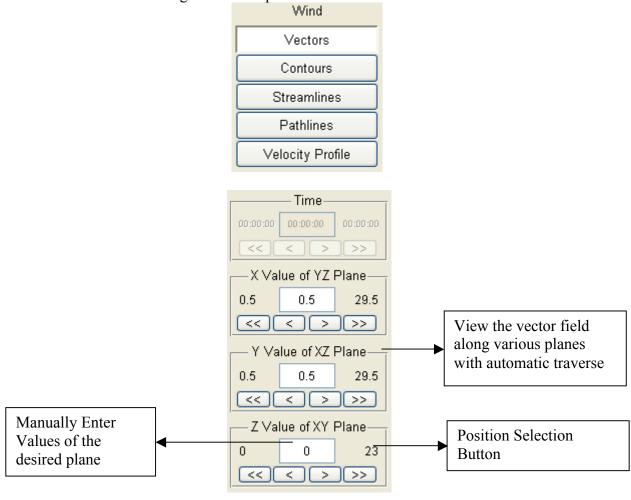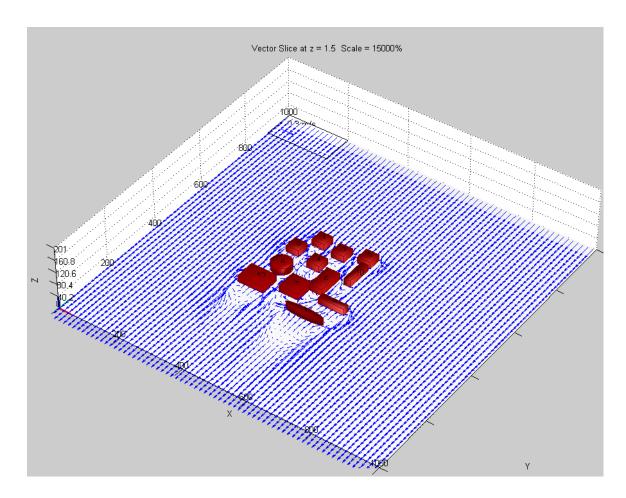
QUIC-URB VISUALIZATIONS

Vectors

To view the vector field along a particular plane, hit the 'Vectors' button and enter the value of the x-y, x-z, or y-z plane or use the 'Position or Time Selection' buttons [>] until the vector field along the desired plane can be seen. This is shown below.

Wind
Vectors
Contours
Streamlines
Pathlines
Velocity Profile

Time
00:00:00   00:00:00   00:00:00
<<   <   >   >>

X Value of YZ Plane
0.5   0.5   29.5
<<   <   >   >>

Y Value of XZ Plane
0.5   0.5   29.5
<<   <   >   >>

Z Value of XY Plane
0   0   23
<<   <   >   >>

View the vector field along various planes with automatic traverse

Manually Enter Values of the desired plane

Position Selection Button

Several plot options apply
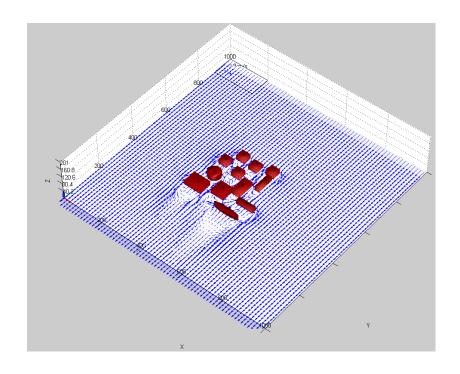
Scale, Vector Spacing and Line Width
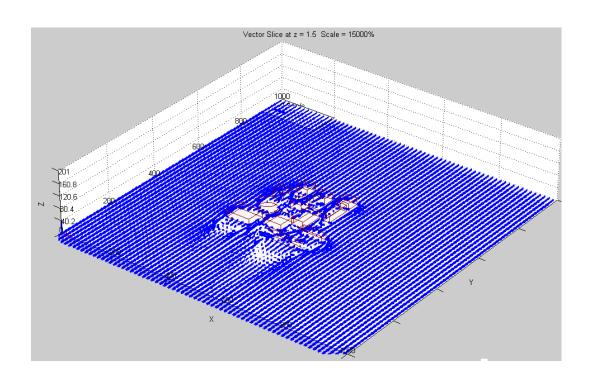
Vector spacing determines the number of grid cells between vector arrows, i.e., a vector spacing of 2 means that 1 arrow is placed every 2 grid cells.

The scale value is multiplied by the vector magnitude to magnify smaller vectors, note that $0 = 1 =$ no scaling

Line width increases or decreases the line width of the vectors in the vector plot. The figures below show the difference between vector plots with Line Width $= 1$ versus Line Width $= 3$.

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Vector Plot with Line Width = 1
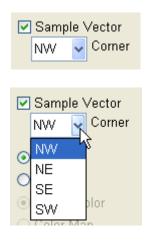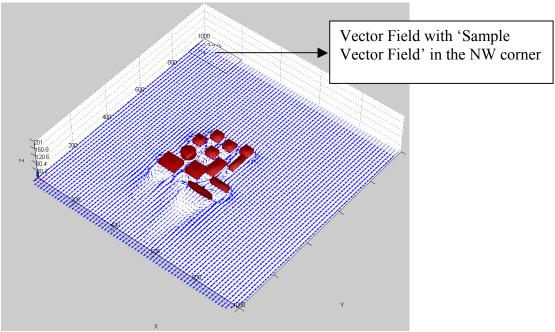
Vector Plot with Line Width = 3

Sample Vector

Selecting the 'Sample Vector' option places a sample vector field on any of the four corners of the vector plot. Deselecting the 'Sample Vector' option does not place a sample vector field. The user can choose to place the sample vector field on any of the four corners, i.e. North-East, North-West, South-East or South-West. This is illustrated in the figures below.

Vector Field with 'Sample Vector Field' in the NW corner
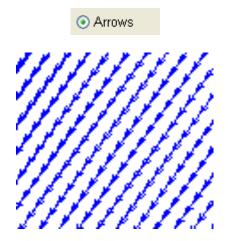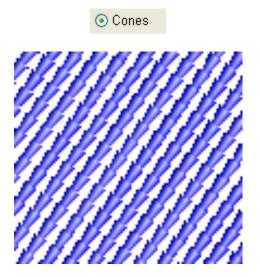
Arrows

Selecting the 'Arrows' option places arrows as vector heads. This is shown below.

Cones

Selecting the 'Arrows' option places arrows as vector heads. This is shown below.
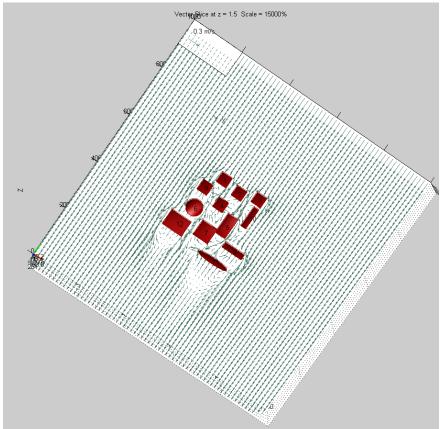
Single Color

The only option for coloring vector arrows is 'Single Color' cones can have a uniform color or be colored by various local quantities. Selecting the 'Single Color' option plots the vector field without any contour levels. That is to say that the color does not represent the magnitude of the velocity. The user has the option of choosing the color of the vector field. To do so, click the color button ▮. This launches the 'Set Color' window. Using this, choose the color of the vectors in the vector plot. This is shown below.
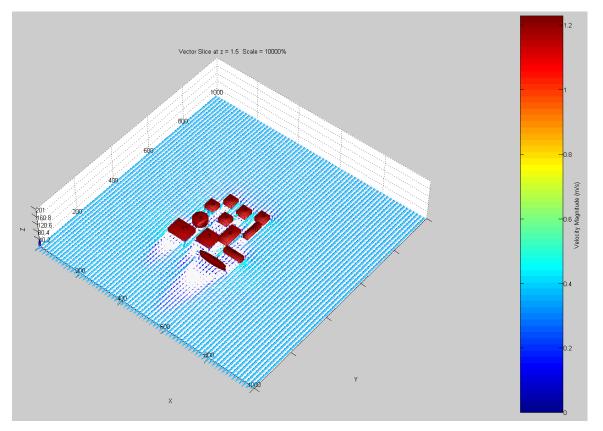
The figure above shows the vector plot with the green color vectors

Note: The 'Single Color' option can be used both the 'Arrows' and 'Cones' options

Color Map

The 'Color Map' option at present works only with the 'Cones' option. Selecting the 'Color Map' option plots the vector field with contour levels. That is to say that the color of the vector field is representative of the magnitude of velocity. This is shown in the figure below.
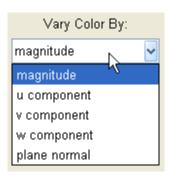
The user has the option of picking colors for the color map. This can be done through the pull down menu as shown below.
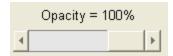
Coloring Cones by Various Quantities
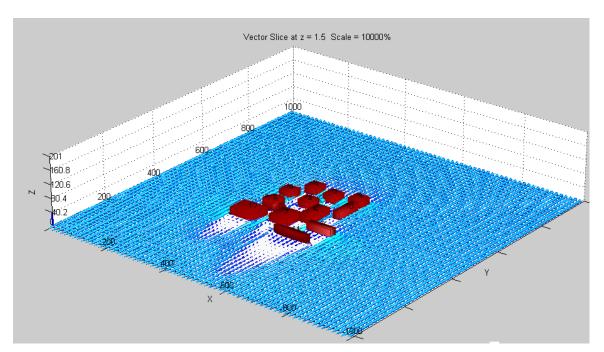
The user has the option of viewing the vector field based in the magnitude of velocity or based on the u, v, or w components of velocity. This can done using the pull down menu as shown below.
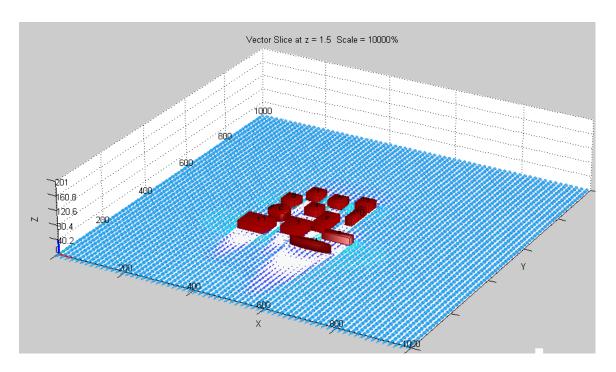
Opacity

The opacity option can be used to add transparency to the vector field. By this it follows that 0% opaque would make the vector field invisible. Opacity can be changed with the slide bar as shown below.
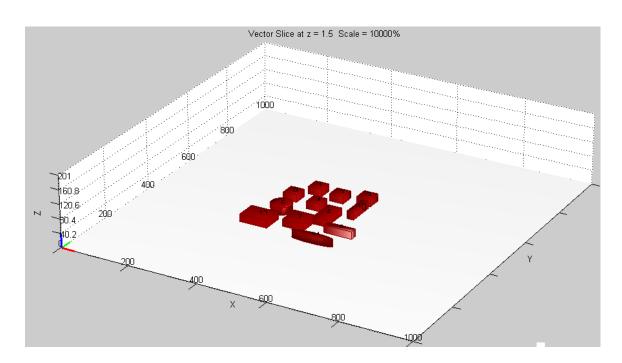
Opacity = 100%
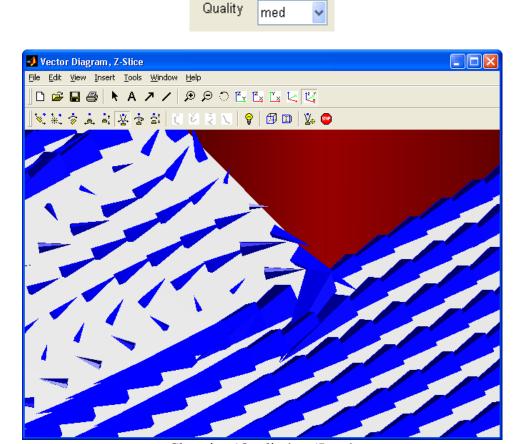
Opacity = 50%
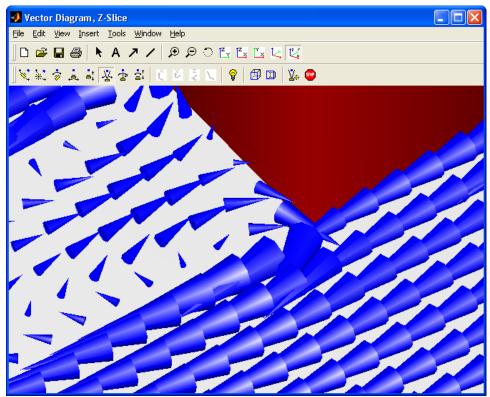
Opacity = 0%

Quality
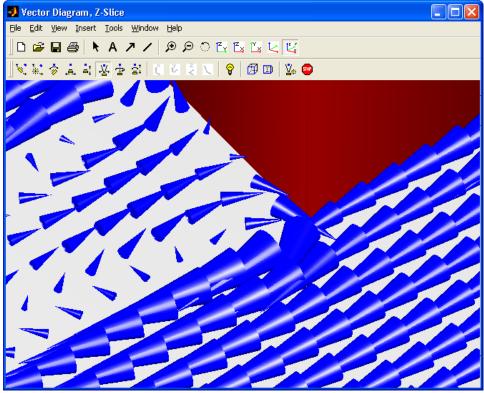
Choosing 'Quality' determines the resolution of the graphics used to display the plot. The 'Quality' pull down menu gives the user three options; of choosing between High, Medium and Low. Though choosing 'high' gives better graphical resolution, it is more time intensive. Choosing 'Low' gives the user the plot faster but with lesser graphical resolution. This is due to the computation being done on the fly. The differences in the plots when each of these options is chosen are shown below.

Choosing 'Quality' as 'Low'
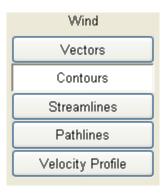
Choosing 'Quality' as 'Medium'
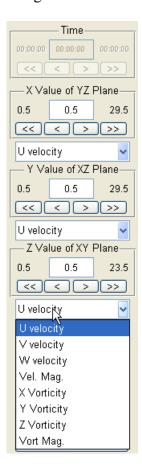
Choosing 'Quality' as 'High'

Contours

The resultant vector field from QUIC URB can be visualized as contour plots by pressing the contour button under QUIC-URB Visualizations
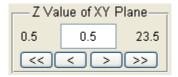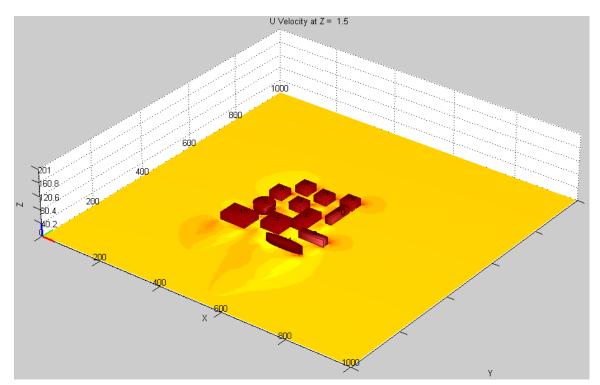
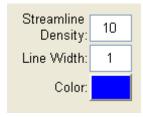VIS-GUI provides the user the option of viewing the contours of all three components of velocities and also the contours of quantities derived from the mean velocity field (vorticity etc). This is depicted in the figure below.

Note: While vorticity is one of the default plot options it is not calculated by default. This is because this can be computationally expensive, particularly for large domains. Instead the vorticity is computed the first time that the user plots the vorticity field and is saved in 'vorticity.mat' for later use. Thus it will likely take much longer to plot vorticity the first time than it will in subsequent attempts. This plot option can also be used to plot the turbulence fields (velocity standard deviations, TKE, friction velocity, dissipation rate, and mixing length) if the 'QP_turbfield' output file option was selected before running QUIC-PLUME.
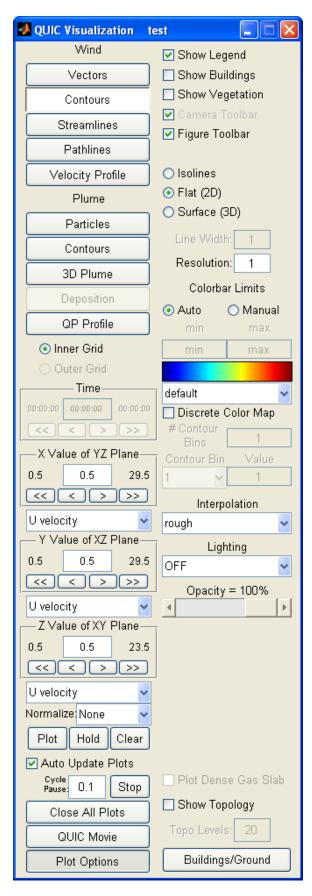
To view the contour plot along a particular plane, enter the value of the x-y, x-z, or y-z plane or use the 'Position Selection' button ⟨ > ⟩ until the contour along the desired plane can be seen. This is shown below.

For enhanced effects, press the 'Plot Options' [Plot Options] button and this brings up a host of options for better visualizing contour plots. This is shown in the figure to the right.
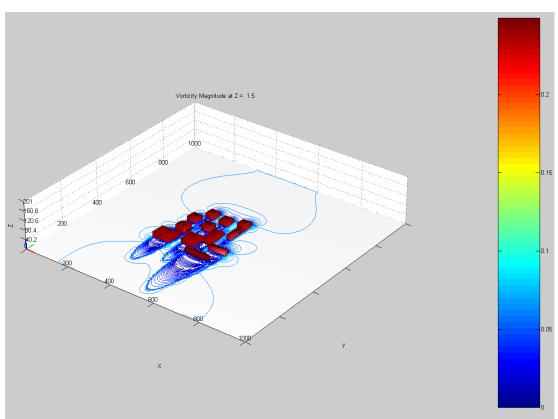
The first three options, i.e. 'Show Legend', 'Show Buildings' and 'Figure toolbar' are the same as the ones described in the previous sections.

Isolines

Selecting the 'Isolines' option draws isolines in the domain for the velocities or their derived quantities. This is shown below.
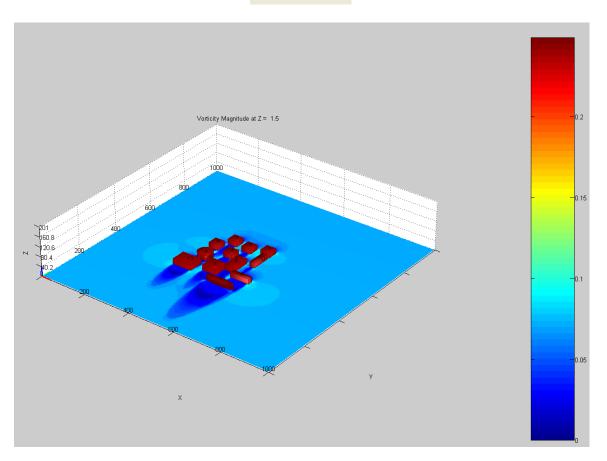
Isolines showing Vorticity Magnitude

Flat (2D)

Selecting the Flat 2D option plots 2D solid contours of velocities or their derived quantities. This is shown below.
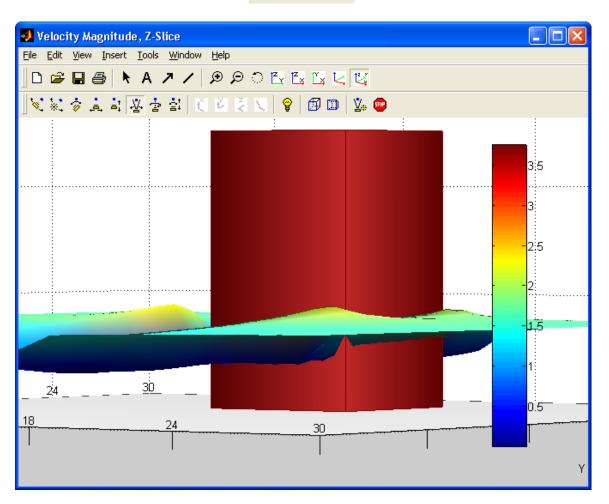
2D Contour Plot of Vorticity Magnitude

Surface (3D)

Selecting the Surface 3D option produces a 3D surface plot of the contours as is shown below.
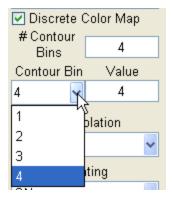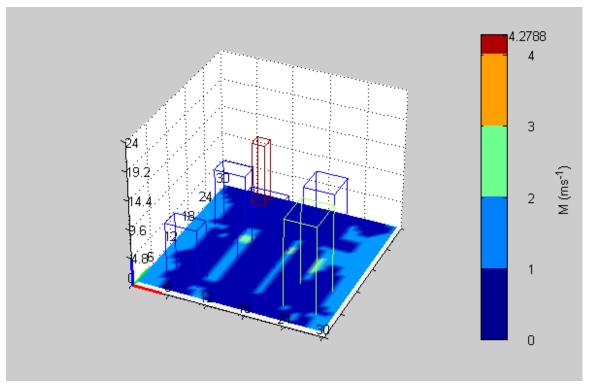
3D Contour Plot of Velocity Magnitude

Discrete Color Map
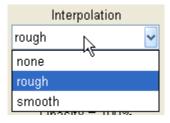
 'Discrete Color Map' gives the user the option of specifying the contours levels. To do so, enter the number of contour bins that have particular value.
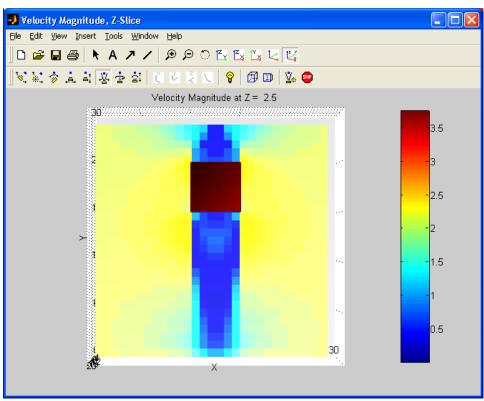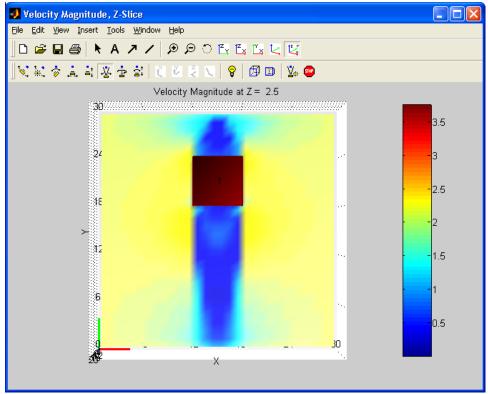
Interpolation

The interpolation option interpolates between the various contour levels and produces smoother contour plots. There are there interpolation options; none, rough and smooth. As was the case with 'Quality - High', choosing 'Smooth' takes longer time for plotting but gives higher graphical resolution. This is illustrated in the plots below
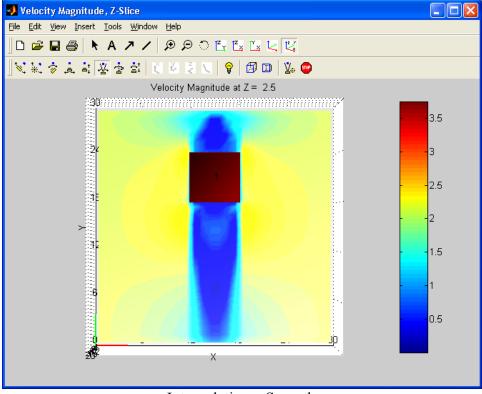
Interpolation - None
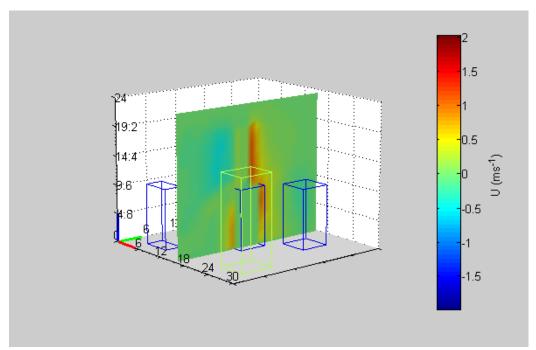
Interpolation – Rough
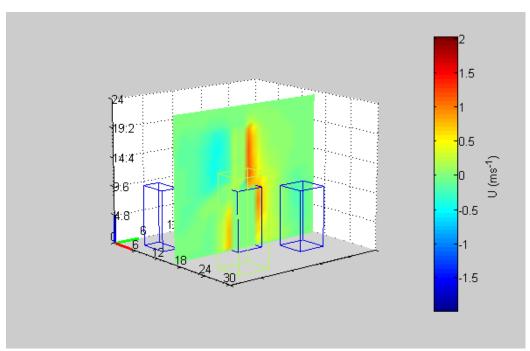
Interpolation – Smooth

Lighting

The lighting used in the 3D plotting functions can often produce distortions from the plotted contours to what is seen in the color bar. Turning off the lighting removes this distortion. Note that smooth interpolation requires lighting to be on.
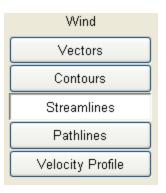
With lighting turned on.

With lighting turned off.

Streamlines

The resultant vector field from QUIC URB can be visualized as streamlines by pressing the streamlines button under QUIC-URB Visualizations

VIS-GUI provides the user the option of viewing the streamlines in various planes. For additional plot options, press 'Plot Options' as was described in the previous sections. This launches a window with additional streamlines plot options. The various plot options for streamlines are shown below.
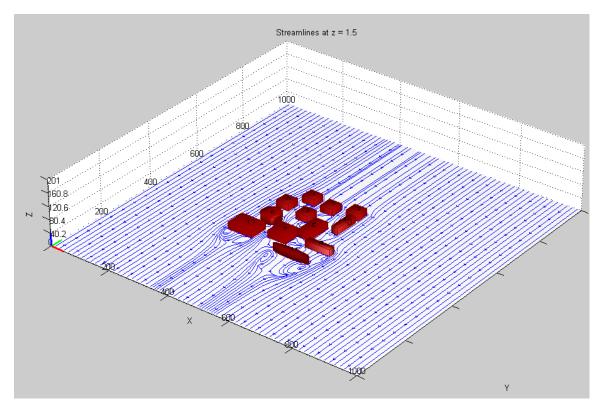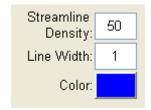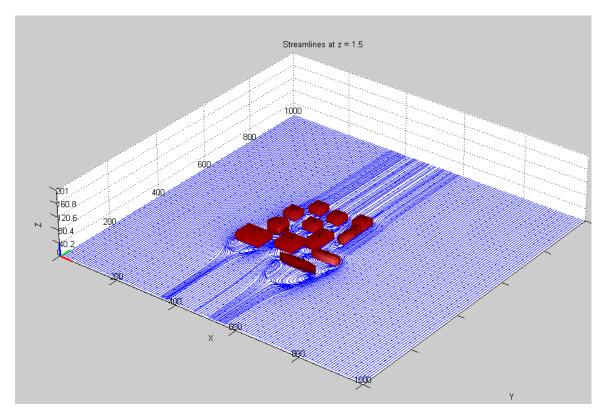
Streamline Density

Streamline Density provides the user the option of increasing or decreasing the density of streamlines in the plots. This is shown below.
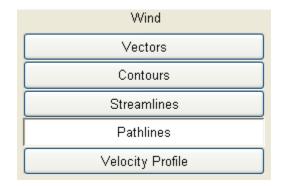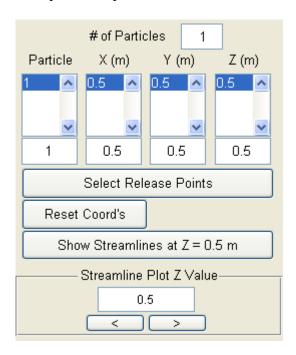
Pathlines

Pathlines of the wind field can be visualized by pressing the pathlines button under QUIC-URB Visualizations

This bring up a window with pathline options

The maximum number of particles that can be released is 64. Enter the number of particles between 1 and 64 in the 'Number of Particles' window

Choose the location of each particle by either entering the x, y and z co-ordinates of the location of choose the 'Select Release Pts' [Select Release Points] button
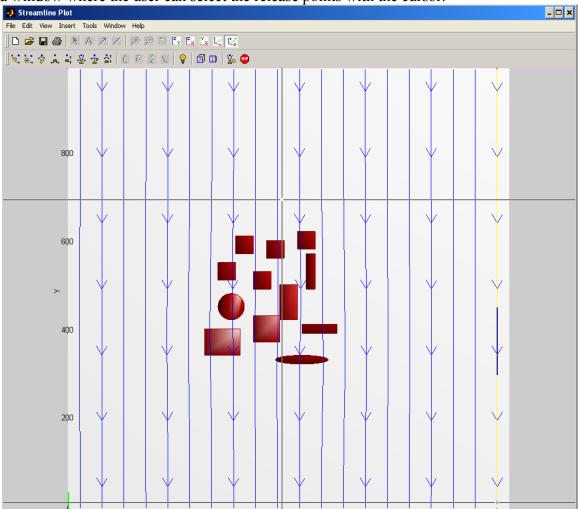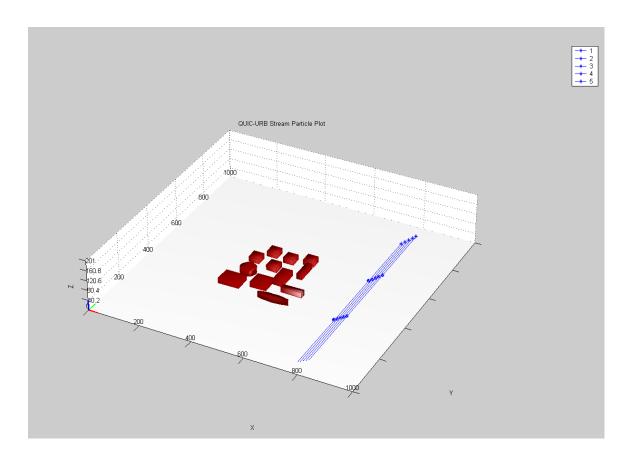
Clicking the 'Select Release Pts' [Select Release Points] button brings up a window where the user can select the release points with the cursor.
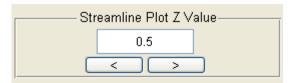
If entering the x, y and z coordinates, press the 'Plot' button [Plot]. This plots the pathlines at the specified locations.
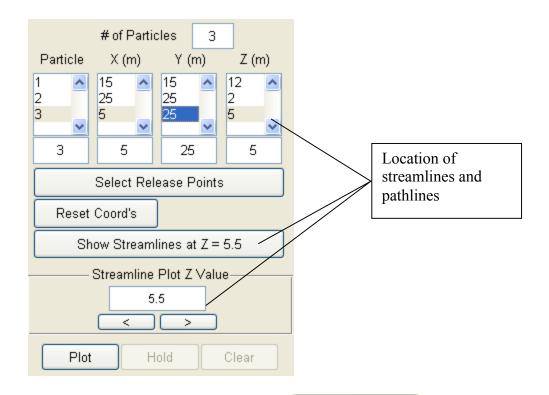
Pathline Plot

To view the streamlines, enter the value of the location of the steamlines in the 'Streamline Plot Z Value' window or use the 'Position location' button to navigate to the desired location
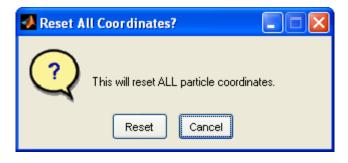
To view the streamlines at the same locations as that of the pathlines, select the location of the pathlines. This by default changes the location of the streamlines to that of the pathlines in the 'Streamline Plot Z Window' and the 'Show Streamlines at Z' button. This is shown below.

Location of streamlines and pathlines

To reset the particle coordinates, click the 'Reset Coord's' button
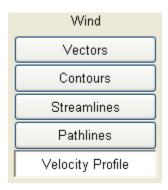
This will bring up a pop up window as shown
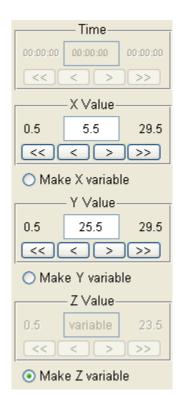
Click on 'Reset' to reset the coordinates

Velocity Profiles

Velocity profiles can be viewed by pressing the 'Velocity Profiles' button..

Line profiles at a particular location and along a particular axis can be viewed by selecting the particular axis. This is shown below.
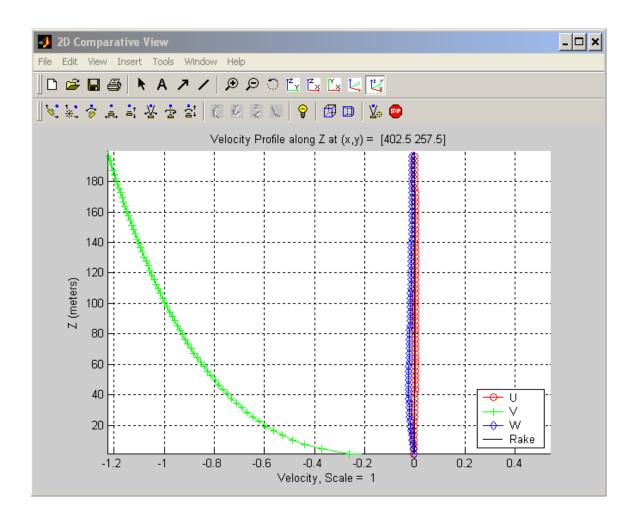
'Making Z variable' plots the velocity profiles with respect to Z axis (vertical direction).
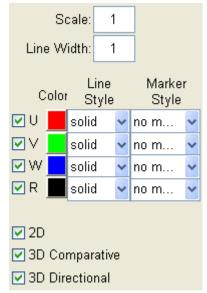
For additional plot options, click the 'Plot Options' button

The figure below shows the velocity profiles at a particular location.

The user can choose to plot any of the three velocity component at a particular location by selecting or deselecting the respective components. For the figure above, all three velocity components were plotted.

Deselecting all the three components and selecting only the Rake ('R') plots the location where the velocity profiles were intended to be plotted.
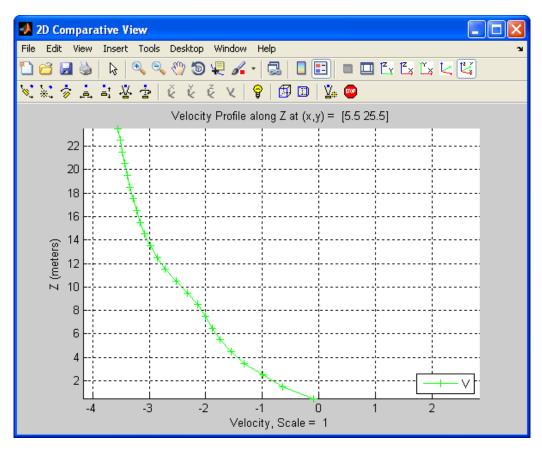
Selecting '2D' plots the velocity profiles on a 2D plane
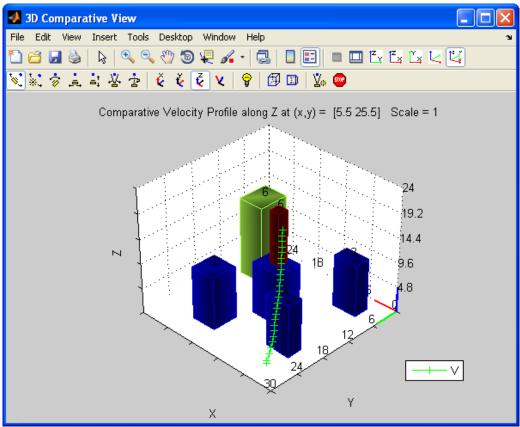
Selecting '3D Comparative' plots the velocity in the 3D domain
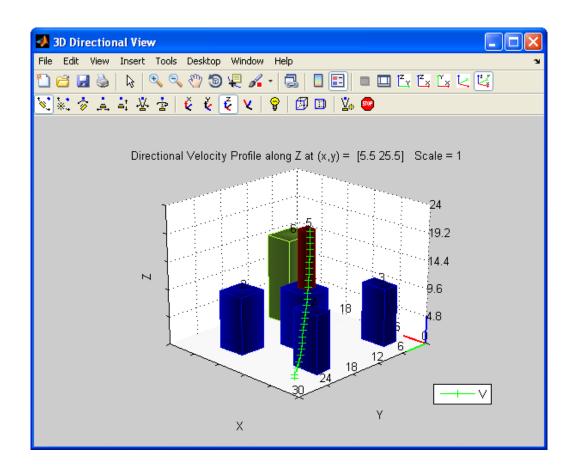
Selecting '3D Directional' gives the user the directional velocity profile

Consider the case where only the 'V' component is being plotted. For this case, the aforementioned plots are shown.
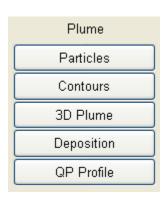
QUIC PLUME VISUALIZATIONS

Below are the toggle buttons corresponding to the QUIC-PLUME data visualizations
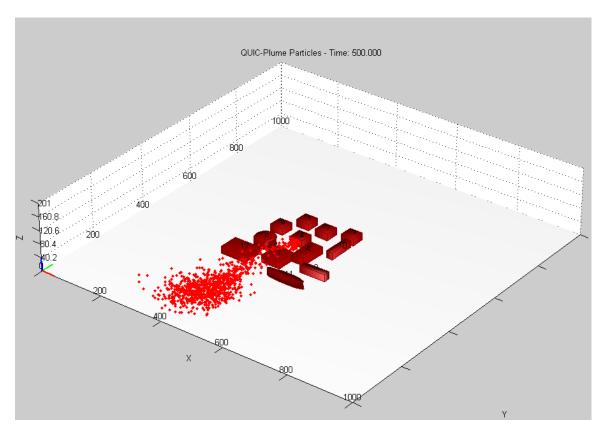
Particles

To view the locations of the particles released at a particular time step, press the 'Particles' button.

The user can select the time at which he / she wishes to see the particle positions by entering the value of time in the 'Time' window or by navigating using the 'Time Selection' buttons ⌐ > ¬.
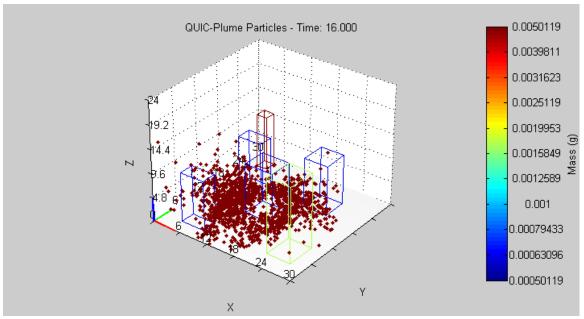

QUIC-Plume Particles - Time: 500.000
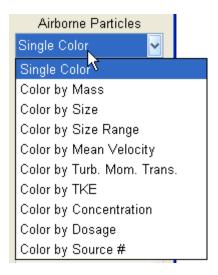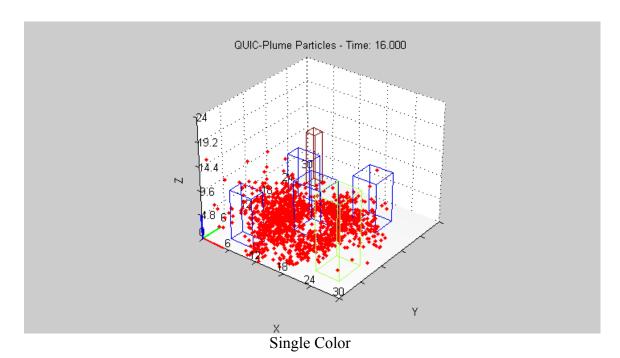
For additional plot options, click the 'Plot Options' button ⌐ Plot Options ¬

Coloring Airborne Particles
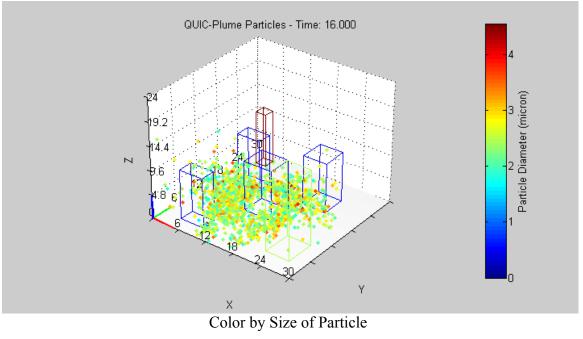
The 'Airborne Particles' option provides the user of visualizing the particles based on various properties. This is illustrated through the figure below.
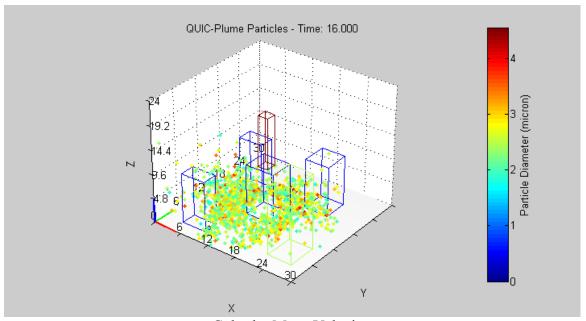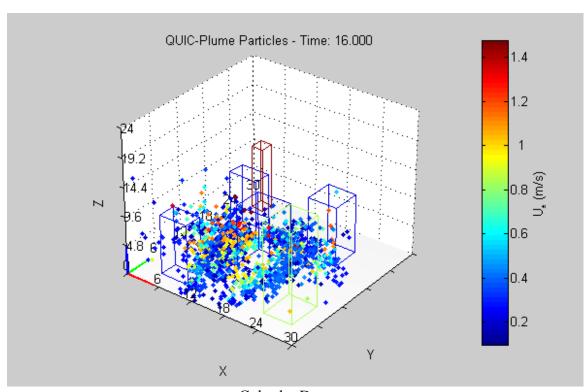

Single Color

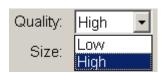Color by Mass of Particle

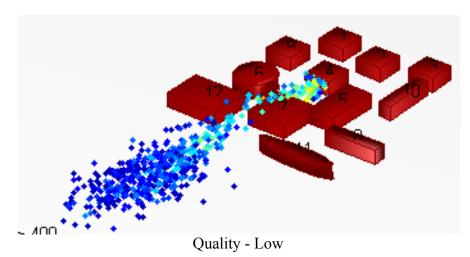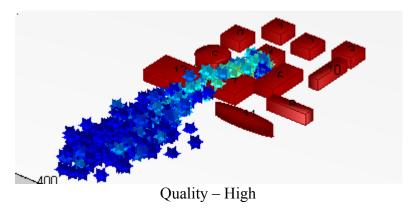Color by Size of Particle

Color by Mean Velocity

Color by Dosage

Quality

The quality option if for enhancing the graphic effects of the plots. Choosing 'High' gives better graphical resolution but takes longer time.
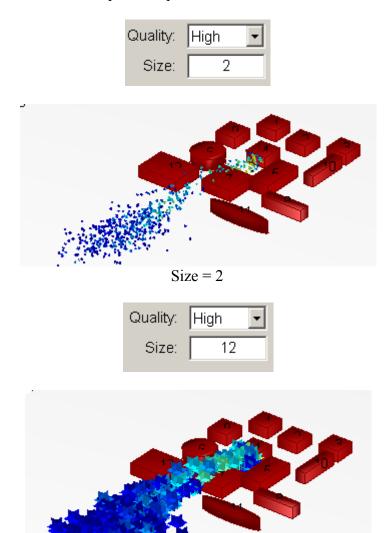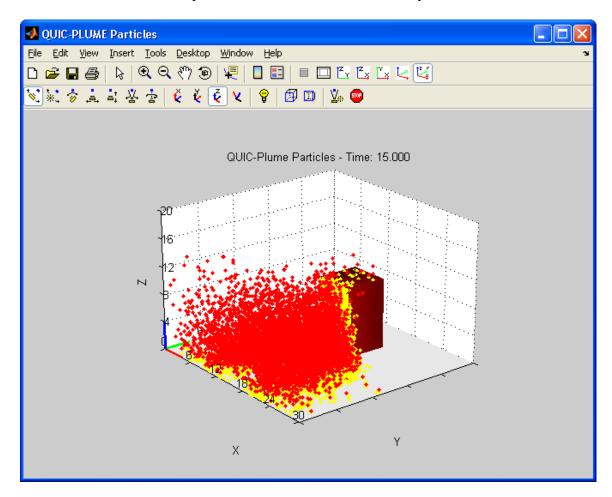

Quality - Low

Quality – High

Size

Size determines the size of the particles plotted.

Size = 2

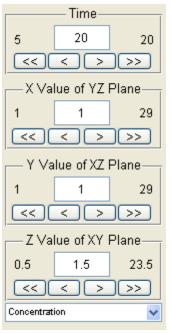Size = 12

Deposited Particles

If the deposition velocity was not set to 0 in the Source Setup GUI, the deposited particles can be plotted with the airborne particles. Currently the deposited particles can only be plotted as a single color. In the plot below the yellow particles are the locations where material has been deposited on the surfaces and the red particles are airborne.
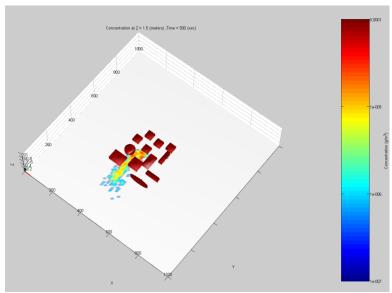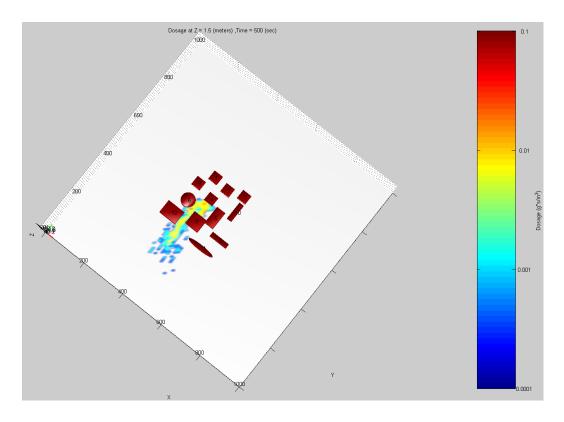
Contours

Results from QUIC-PLUME can be visualized as contour plots. To do so, click the 'Contours' button

Contours of Concentrations, Dosages and Thresholds can be plotted at different time intervals and along various planes by selecting or deselecting the various options shown below.
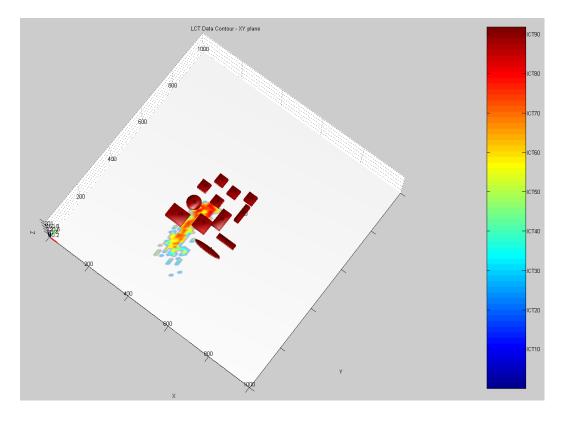

Contour of Concentration along the X-Y plane

Contour of Dosage along the X-Y plane

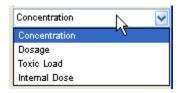Contour of LCT levels along the X-Y plane

For additional plot options, click the 'Plot Options' button [Plot Options]

This brings up a window that has the additional plot options for viewing contour plots using QUIC PLUME. This is shown to the right.
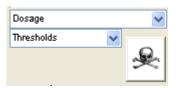
The popup menu just below the position controls selects the source data that is to be displayed: concentration, dosage, toxic load, or internal dose.

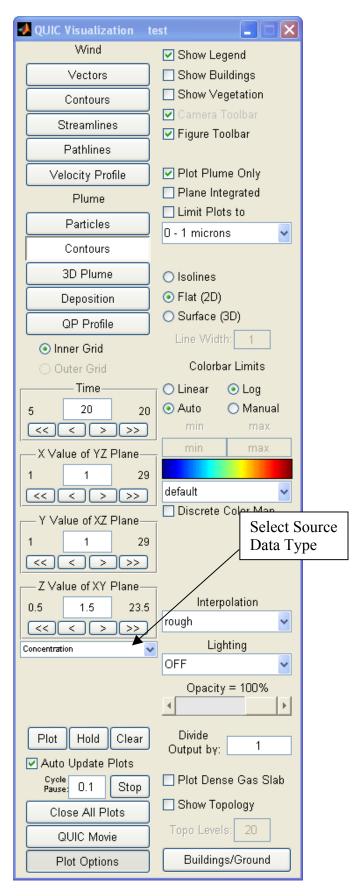Data types other than concentration can be plotted by discrete thresholds or probit slope values in addition to plotting just the data.

If discrete thresholds or probit slope options are selected the Toxicity Data Editor button becomes active.
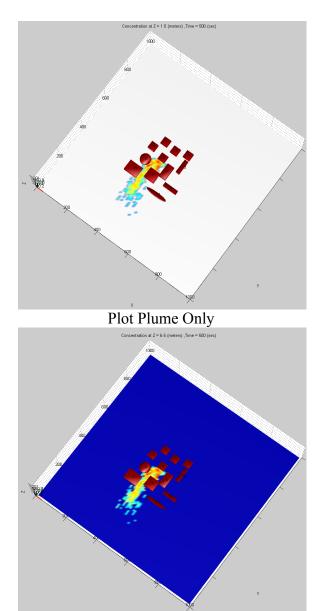
The threshold levels and probit slope values can be modified from the Toxicity Data Editor without having to rerun QUIC-PLUME since this is a post-processing step.

Plot Plume Only
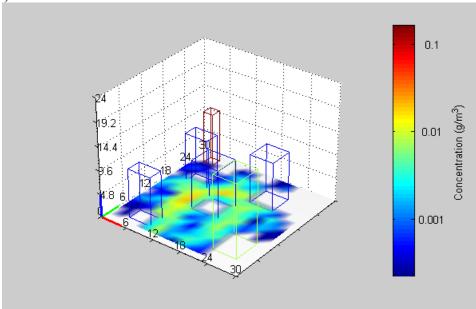
Selecting the 'Plot Plume Only' plots the plume alone. Deselecting it adds a color to the surface. This is shown below.
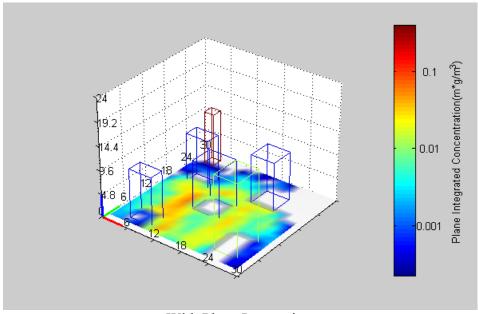
Plot Plume Only

Deselecting Plot Plume Only

Plane Integrated

Selecting the 'Plane Integrated' option integrates the contours of concentration or dosage or thresholds either laterally, longitudinally or vertically. That is to say that if the user wants to view the plane integrated concentration along the X-Y plane, it would be the result of all the concentrations integrated along the vertical planes (along all the columns).

Without Integrating into the Plane

With Plane Integration

Plotting Discrete Threshold Contours

Selecting 'Thresholds' in contour plot type popup menu will produce a plot of the selected plume data type (dosage, toxic load, or internal dose) using the discrete thresholds defined in the Toxicity Data Editor. Below is an example of an airborne dosage discrete threshold plot.
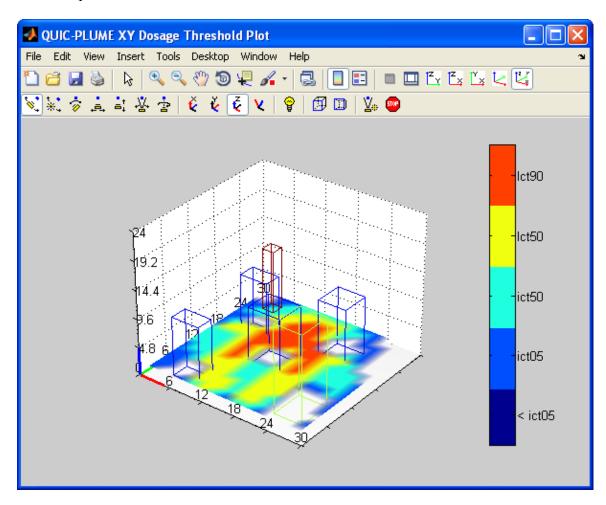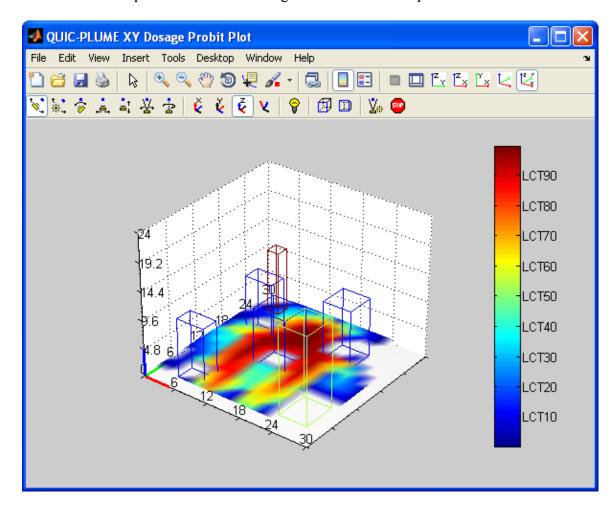
Plotting Probit Slope Contours

Selecting 'Probit Slope' in contour plot type popup menu will produce a plot of the selected plume data type (dosage, toxic load, or internal dose) using the selected continuous probit slope dose response curve defined in the Toxicity Data Editor. The probit slope response curve is selected from a popup menu below the plot type popup menu.
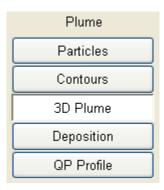
Below is an example of an airborne dosage discrete threshold plot.
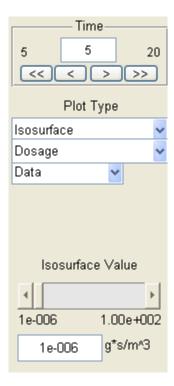
The other plot options are similar to those described in the previous sections

3D Plume Visualization

To view the plume in 3D, press the '3D Plume' button.
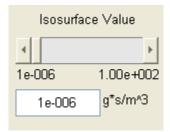
3D plume visualizations can be either isosurfaces, 2D textured smoke slices or 3D smoke volumes. The type of plot is selected using the popup menu and the type of data visualized is selected using the radio buttons seen below. Select a time at which the plume needs to be plotted by either entering the values manually or by using the time selection button ⟩
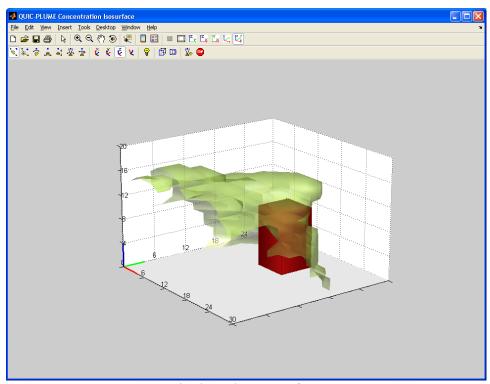
Isosurface
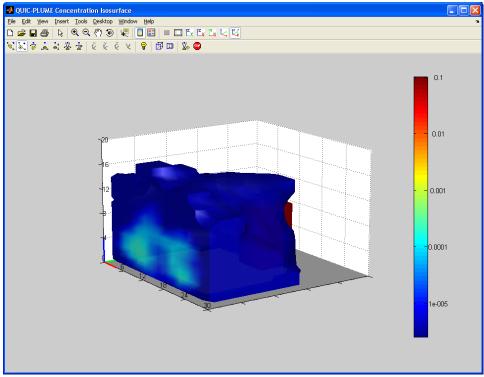
If the isosurface plot type is selected the isosurface value slider and edit box will be enabled.

For additional plot options, click the 'plot options' button. Similar to contours, the opacity and quality of the isosurface can adjusted. In addition, when the color map option is selected for an isosurface caps are added where the plume leaves the domain.
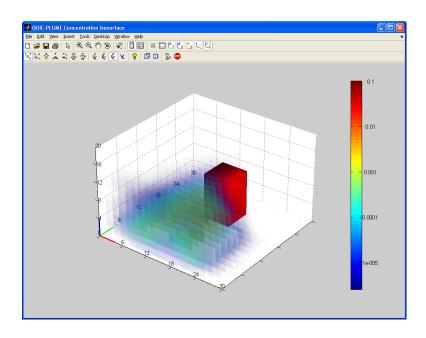
Single Color Isosurface
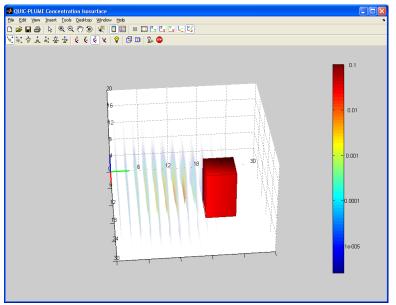
Color Mapped Isosurface with end caps

2D textured Smoke Slices

The 2D textured smoke allows the user to see the entire plume at once rather than a single isosurface. The 2D textured smoke option produces color mapped slices of the plume. The code will chose the orientation of the slices for optimal visualization of the plume given the current orientation of the figure. If the plot is reoriented after plotting the 2D slices will be evident as seen below.
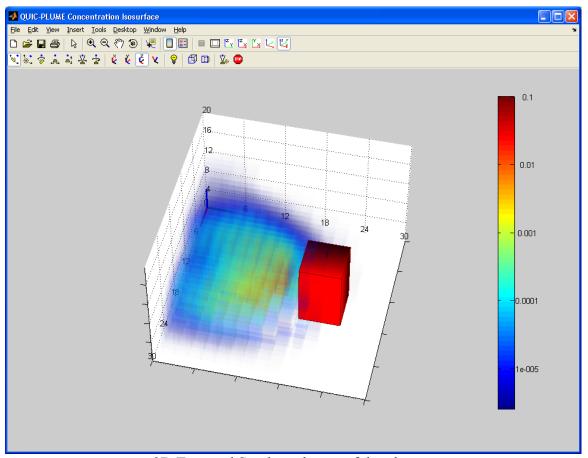
2D textured smoke plot before reorientation.

2D textured smoke plot reoriented to show the slices of the plume.

3D Textured Smoke Volumes
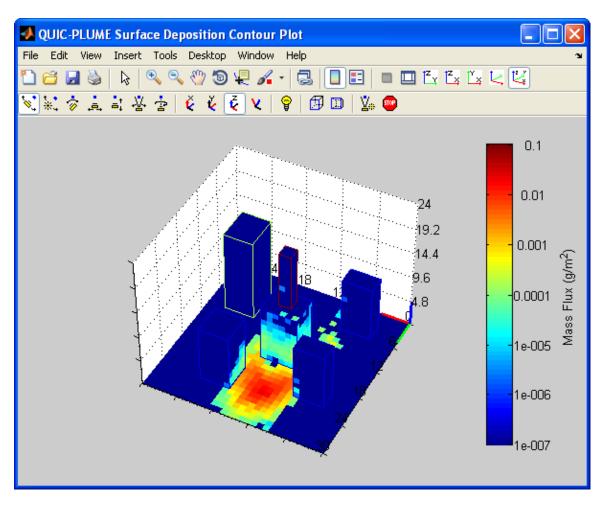
This option is very similar to the 2D textured smoke slices but it is not orientation dependent. It is, however, more computationally intensive and does not produce as vibrant of colors because there are more transparent patches used to produce the volumes.

3D Textured Smoke volumes of the plume.

Surface Deposition
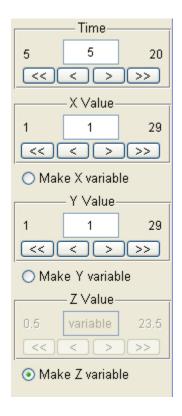
If the deposition velocity was not set to 0 in the Source Setup GUI then the surface deposition plot will be available. Similar to the airborne concentration/dosage fields, one can either plot the surface fluxes or thresholds. The thresholds can be discrete or can be continuous through the use of probit slope population response curves. An example of a surface deposition plot is shown below.

QP Profile

QP Profile enables the users view the concentration profiles in 2D and 3D planes

Line profiles of concentration at a particular location and along a particular axis can be viewed by selecting the particular axis. This is shown below.
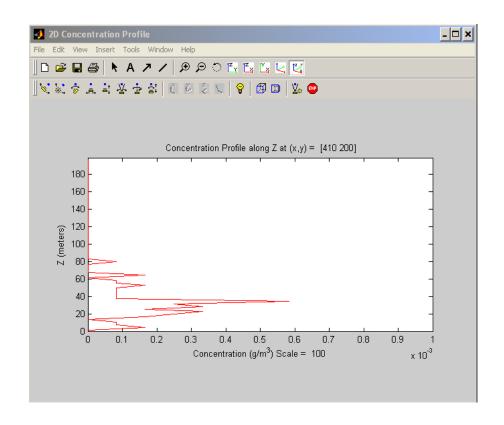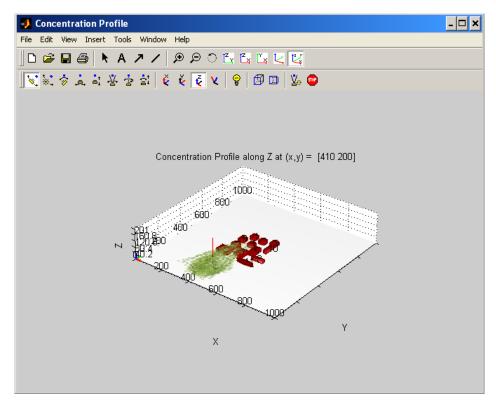
'Making Z variable' plots the concentration profile with respect to Z axis (vertical direction). For additional plot options, click the 'Plot Options' button

Selecting '2D Profile Plot' plots the concentration profile in the 2D plane

Selecting '3D Profile Plot' plots the concentration profile in the 2D plane
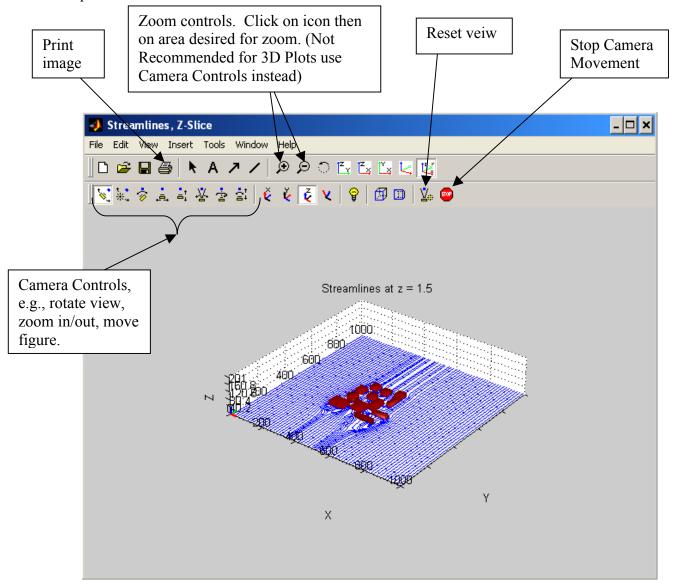
This is shown below
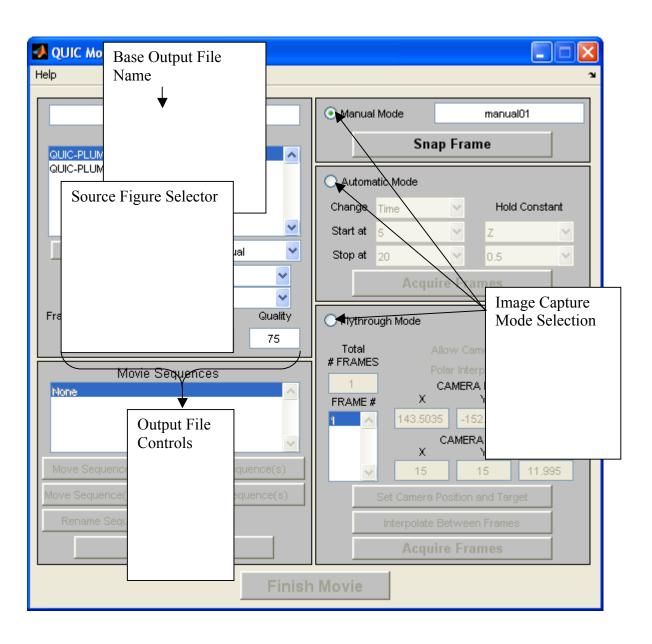
Plot controls

The example streamline figure below shows the different options for manipulating the plot. The controls are standard Matlab features.

Zoom controls. Click on icon then on area desired for zoom. (Not Recommended for 3D Plots use Camera Controls instead)

Print image

Reset veiw

Stop Camera Movement

Camera Controls, e.g., rotate view, zoom in/out, move figure.

QUIC Movie GUI

QUIC Movie GUI is accessed by pressing the QUIC Movie button

at the bottom of the Visualization GUI. This GUI can be used to save animations of the graphical output of the QUIC Visualization GUI as animated GIF files, AVI movie files or numbered .jpg, .png, .bmp, or .tif files. The QUIC Movie GUI is shown below.

Image Capture Modes

There are three basic modes for capturing animations of QUIC data plots produced by the Visualization GUI: Manual, Automatic, and Flythrough. Each of these modes will be discussed in detail below.

Manual Mode

Pressing the 'Snap Frame' button in Manual mode simply captures a single image from the figure selected in Source Figure list box and adds it to the image sequence whose name is in the edit box above the 'Snap Frame' button. Editing the name of the current sequence will cause any subsequent image captures to be stored in a new sequence with the new sequence name. In manual mode all modifications to the image are performed outside of the Movie GUI.
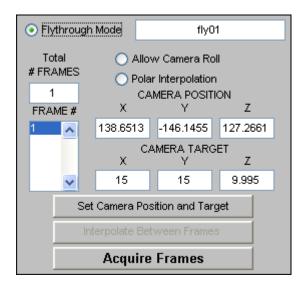
Sequence Name

Automatic Mode

Automatic mode can be used to automatically capture images while [ ] data (such as changing time or position). When the automatic captu[ ] the automatic controls shown below become active.

Some plot types have two variables that can be modified such as contour plots which may have multiple time steps and plane positions. Other plots have only a single variable that can be changed such as particle p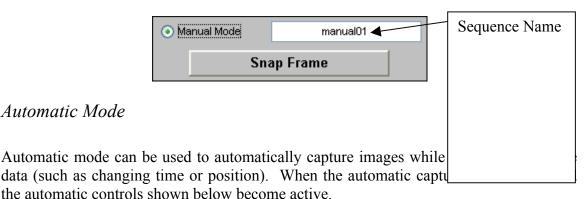lots where time is the only variable. Only one variable may be cycled through at a time. If two variables are available for the selected plot type, select the variable to cycle through with the pop-up on the upper-left hand side of the automatic controls. Then select the start and end values for that variable and select the value of the variable that is to be held constant. After setting all of the controls, initiate the frame capturing process by pressing the 'Acquire Frames' button. The plot will automatically cycle through the selected values and add the acquired frames to the sequence name found in the edit box.

Flythrough Mode

The perspective of the 3D plots is defined by the camera position (the location of the observer) and camera target (the point which corresponds to the center of the figure). Flythrough mode allows the user to automatically modify the camera position and target over a user-specified number of frames in order to simulate flying through the 3D model. The flythrough controls are shown below.

A flythrough frame sequence is produced by setting the total number of frames for the sequence in the edit box in the upper-left hand corner. The path of the 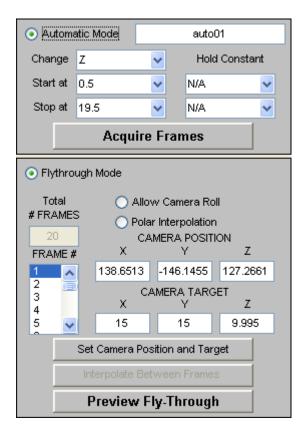camera position and target can either be set manually for each frame or can automatically be interpolated between beginning and ending locations. The camera position and target can be set manually set with the edit boxes or can be captured from the figure itself using the 'Set Camera Position and Target' button. Select a frame to use as the starting position using the frame number list box on the left. Manipulate the camera target and position using the camera controls found at the top of the figure window and save the current camera target and position by pressing the 'Set Camera Position and Target' button. Select an ending frame with the frame number list box and manipulate the camera position and target with the camera controls to the ending position and press the 'Set Camera Position and Target' button again to save the end location. Then select the frames to interpolate between by holding the 'Ctrl' button on the keyboard and left-clicking on the beginning and ending frames in the frame number list box. Once the camera target and position for the beginning and ending frames have been set and the frames have been selected in the list box, press the 'Interpolate Between Frames' button to automatically interpolate between the beginning and ending positions in the frames between the two selected frames. The interpolation defaults to being linear in Cartesian position between the points but selecting the 'Polar interpolation' radio button will cause the interpolation to be linear in radius and angle of the camera position relative to the target. The upwards vector of the camera position defaults to being parallel with the z-axis but this can be modified by activating the 'Allow Camera Roll' radio button. After the camera position

and target paths have been defined press the 'Acquire Frames' button to capture the frames and add them to the sequence name in the edit box at the top of the controls.

Automatic Mode with Flythrough
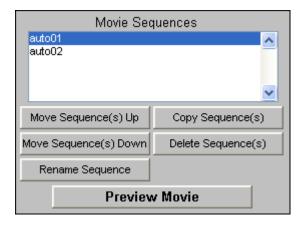
The automatic and flythrough frame capture modes can be used at the same time to cycle through the plot variables and change perspective at the same time. When both automatic and flythrough modes are selected the controls appear as shown below.

The flythrough controls work in the exact same way but the number of frames is determined by the start and stop values of the variable that is to be cycled through. The 'Preview Fly-Through' button can be used to check the paths of the camera position and target without capturing the images and saving them to the sequence in the edit box.
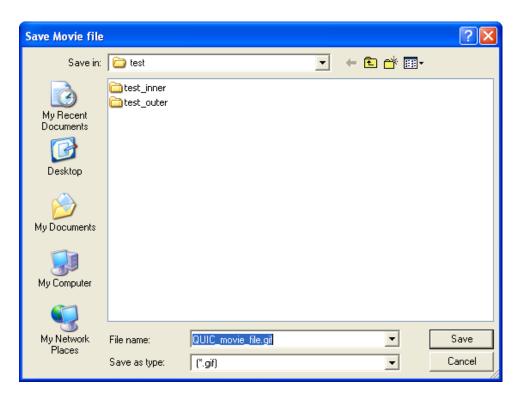
Sequence Control

After at least one sequence has been captured the sequence controls become active as shown below.

Sequences can be copied, deleted, and reordered to produce the desired movie. After manipulating the sequences, select the desired sequences and press the 'Preview Movie' button. This will replay the selected frame sequences in a new figure.

Press the [Finish Movie] button at the bottom of the GUI will prompt the user to save the animation in the selected file format.
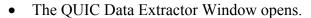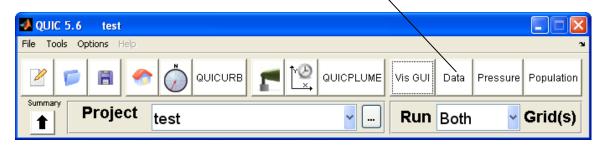
DATA EXTRACTOR
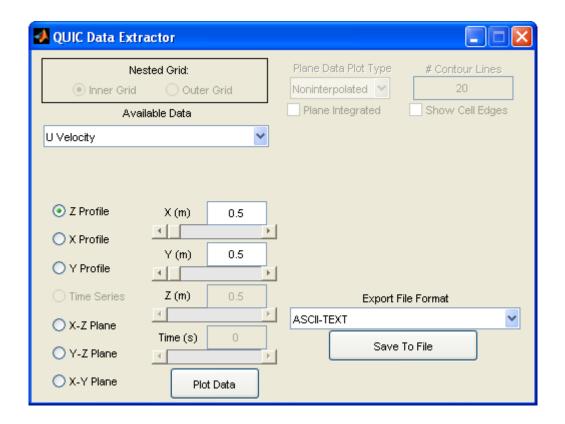
QUIC Data Extractor

The user has the option to output concentration data in column format. Vertical, horizontal, and time series profiles can be saved, in addition to a plane of data. The text output option is useful when wanting to compare model results to experimental data, for example.
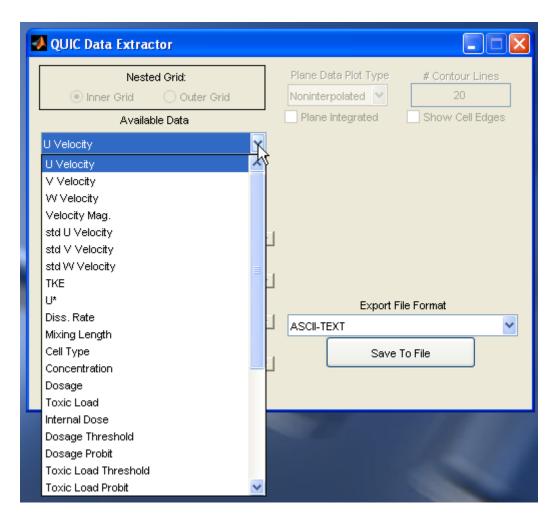
- In the main QUIC window select 'Data Extractor'
- The QUIC Data Extractor Window opens.

- The Data Extractor window has the 'Available Data' option. Using the 'Available Data' pull down menu shows the data that can be plotted and saved.

- After selecting certain flow parameter, it can either be plotted using the 'Plot Data' option or it can be saved using the 'Save to File' option.
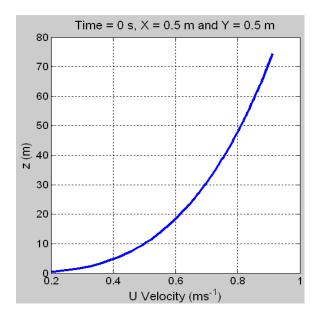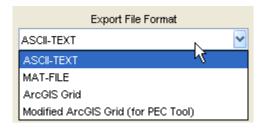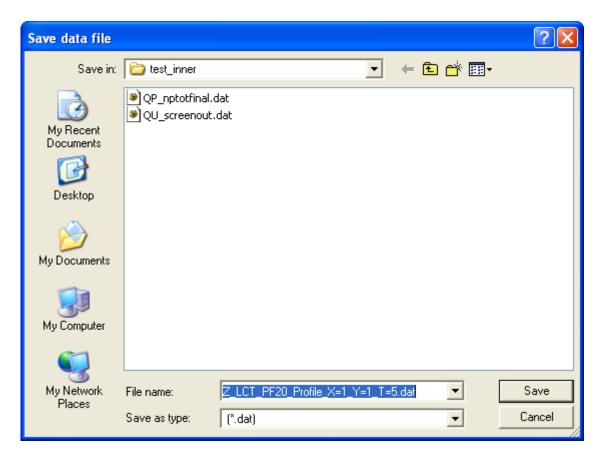
Figure shows the 'U' velocity plotted using the 'Plot Data' option
- The data can be saved in three formats. They are:
  - ASCII
  - MAT files
  - ArcGIS Grid
  - Modified ArcGIS Grid (for ArcGIS PEC Tool)
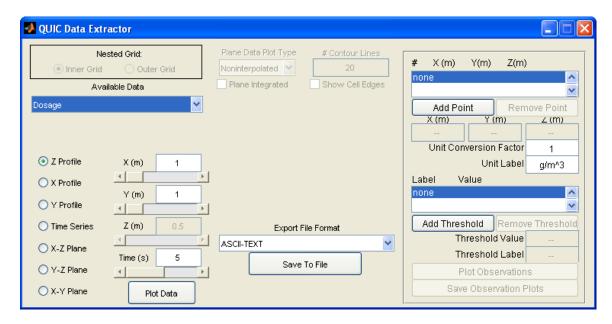
- Select any format and press the 'Save to File' button
- On pressing the 'Save to File' button, the user will be a directed to folder where he/she would like to save the files
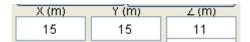
Make selections for desired data output and press "Save" button. The popup window for naming the file opens. The default filename contains descriptive information on the profile or planar coordinates.

Plume Observations
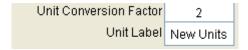
If a raw plume data type is selected (e.g., concentration, dosage, toxic load, or internal dose) then the plume observation portion of the Data extractor becomes visible.
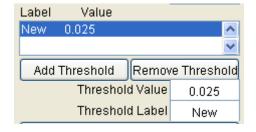
From here several observation points can be defined and saved for later use. Observation points are added by pressing ![Add Point]. After a point has been the location of the observation point must be defined. This is done by entering the desired observation location in the position edit boxes.

The units of the observation plots can be changed by entering a conversion factor and modifying the units string.
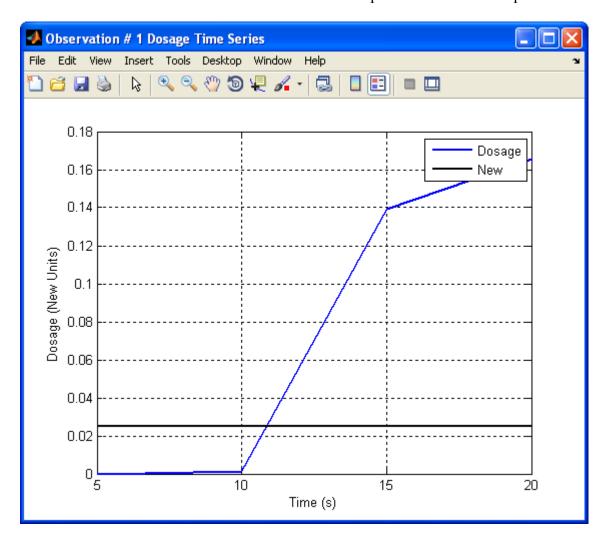
Thresholds can also be added to the observation plots by pressing ![Add Threshold] and defining the threshold value (in the new converted units) and adding a threshold label.

All of the observation plots can now be plotted simultaneously by pressing
[Plot Observations] . Below is an example of the observation plots.
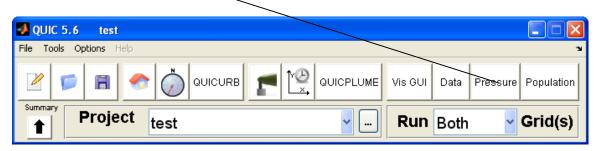
Alternatively, all of the plots can be saved to jpg files simultaneously by pressing
[Save Observation Plots] .
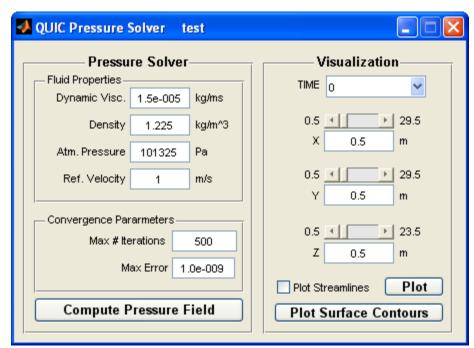
PRESSURE GUI

QUIC Pressure Solver

- Selecting 'Pressure GUI' from the main QUIC window launches the QUIC Pressure Solver

- Various fluid properties such as the dynamic viscosity and density can be specified in the window to the left.
- The user can specify the maximum number of iterations over which the Pressure Poisson Equation should be solved. The default value is 500.
- The user can also specify the threshold for maximum error. The default maximum error is 1e-9.
- After setting all the parameters press the **Compute Pressure Field** button at bottom of the GUI.
- The QUIC Pressure Solver solves the Pressure Poisson Equation for the given domain and computes the pressure field.

- Visualization options are found at the right of the GUI.

- To view the pressure contours along a particular plane, enter the value of the plane (X, Y, or X) or scroll with the sliders until the pressure field along the desired plane can be seen.
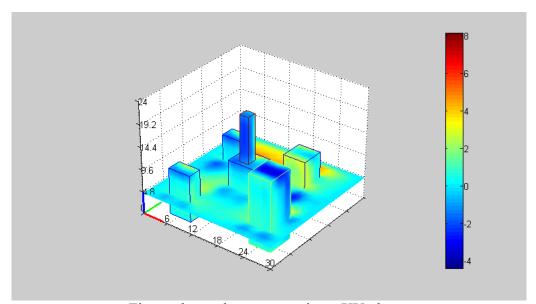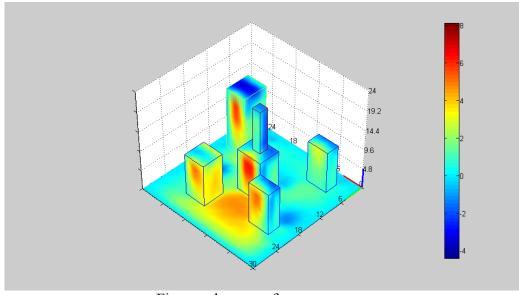
Figure shows the pressures in an XY plane.

- To view the pressure field on the building surfaces, choose **Plot Surface Contours** .

Figures shows surface pressures.

- To view the streamlines along with the surface pressure contour, select the ✅ Plot Streamlines option.
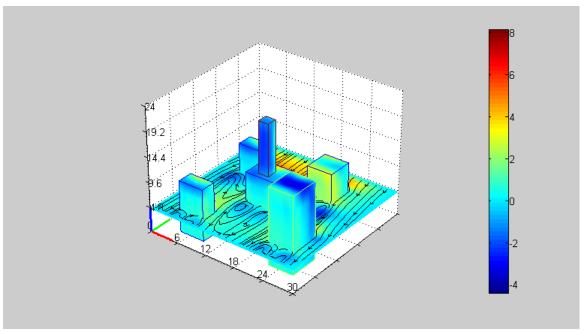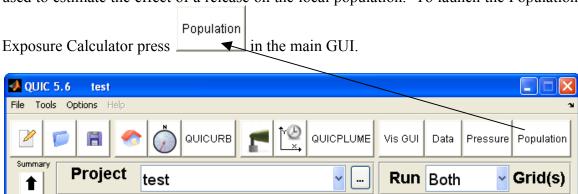
Figure shows streamlines plotted along with the surface pressure contour

- In case multiple time averaged velocity profiles were input through the MET Generator, the pressure fields for the different inflow velocity fields can be seen by using the TIME 0 option.
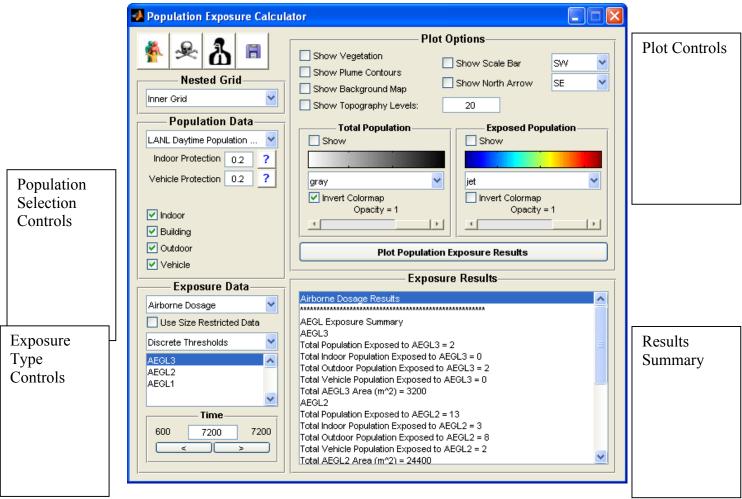
Population Exposure Calculations

Population Exposure Calculator

If the project has been properly georeferenced and the domain is within the lower 48 States, the daytime and nighttime population databases that are included in QUIC can be used to estimate the effect of a release on the local population. To launch the Population Exposure Calculator press [Population] in the main GUI.
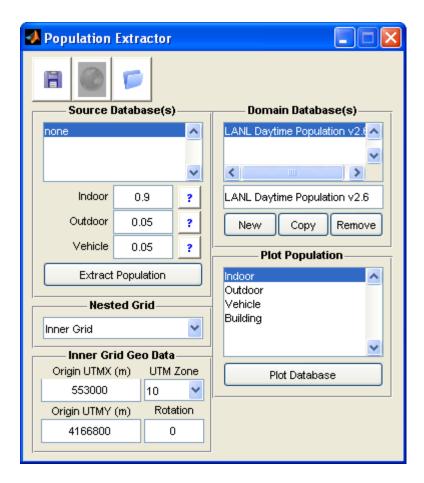
We will use an event reconstruction from an accidental release of ammonia in San Francisco, CA sometime before 5:45 am PDT to demonstrate these capabilities.

Population Exposure Calculator

Plot Controls

Plot Options

- [ ] Show Vegetation
- [ ] Show Plume Contours
- [ ] Show Background Map
- [ ] Show Topography Levels: 20
- [ ] Show Scale Bar
- [ ] Show North Arrow

SW
SE

Nested Grid

Inner Grid

Population Data

LANL Daytime Population ...

Indoor Protection 0.2 ?
Vehicle Protection 0.2 ?

- [x] Indoor
- [x] Building
- [x] Outdoor
- [x] Vehicle

Total Population

- [ ] Show

gray
- [x] Invert Colormap
Opacity = 1

Exposed Population

- [ ] Show

jet
- [ ] Invert Colormap
Opacity = 1

Plot Population Exposure Results

Population Selection Controls

Exposure Type Controls

Exposure Data

Airborne Dosage

- [ ] Use Size Restricted Data

Discrete Thresholds

AEGL3
AEGL2
AEGL1

Time

600   7200   7200
<   >

Exposure Results

Airborne Dosage Results
****
AEGL Exposure Summary
AEGL3
Total Population Exposed to AEGL3 = 2
Total Indoor Population Exposed to AEGL3 = 0
Total Outdoor Population Exposed to AEGL3 = 2
Total Vehicle Population Exposed to AEGL3 = 0
Total AEGL3 Area (m^2) = 3200
AEGL2
Total Population Exposed to AEGL2 = 13
Total Indoor Population Exposed to AEGL2 = 3
Total Outdoor Population Exposed to AEGL2 = 8
Total Vehicle Population Exposed to AEGL2 = 2
Total AEGL2 Area (m^2) = 24400

Results Summary

Population Extractor

If population has not been added to the project you must first press [icon] to launch the Population Extractor.
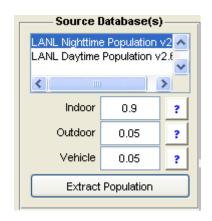
The Population Extractor will retrieve the population that pertains to the specific geographic area of the QUIC domain(s). As such, this can only be done if the project has been properly georeferenced. If the domain(s) have yet to be georeferenced, this information can be added now usning the controls in the lower left-hand corner of the Population Extractor.

Press to choose a database to extract the population data from, daytime or nighttime. Both daytime and nighttime databases can be loaded at the same time in the event that the user desires to add both to the project. This will prompt the user to open database file(s) from the *GISdata* subdirectory in the QUIC installation.
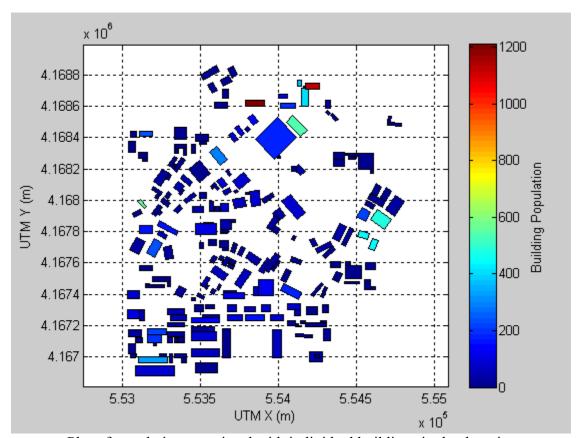
Once the database(s) have been selected and loaded into the GUI the 'Source Database(s)' list will be populated with the selected database(s).
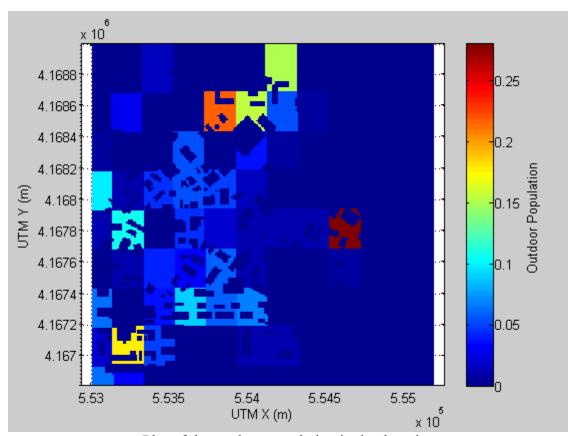
Press the help buttons at the side of the population location fraction edit boxes to receive suggestions regarding the various fractions. Once all of the population fractions have been defined press to extract the data to the collecting boxes and buildings. The LANL population databases included with QUIC consist of grid cells that are approximately 250 meters on a side. The Population extractor will attribute the indoor population to any buildings found within a population grid cell by building volume. Population cells without any buildings in them (usually due to these

buildings not being resolved) have the indoor population evenly distributed to an indoor dataset throughout the collection boxes that pertain to that population cell. Outdoor and vehicle populations are distributed evenly throughout all open collection boxes in the population grid cell.

Press [Plot Database] to plot the selected portion of the population. Examples of the population plots are shown below:

Plot of population associated with individual buildings in the domain.

Plot of the outdoor population in the domain.

Calculating Exposed Population

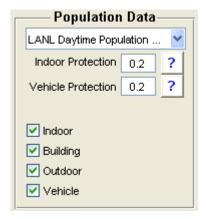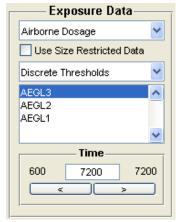Once population data has been added to the project, use the population selection tools to determine which population groups to include:
- Indoor (not associated with individual buildings)
- Building specific
- Outdoor
- Vehicle

The exposure data from the infiltration model will be used to calculate the exposures to population to individual buildings, so the infiltration model (which is off by default) must be turned on to get an accurate population exposure calculations when there are buildings in the domain. For the indoor population that has not been associated with individual buildings and the population in vehicles a dose reduction factor is used to account for the protection that the building or vehicle provides. This is a gross simplification of the actual processes which are better modeled by the infiltration model. In the example shown above the individuals that are indoors (but not associated with individual buildings) and in vehicles will only receive 20% of the outdoor dosage at that same location.

Now that the portions of interest from the population database have been selected the exposure data must be chosen.

The type of exposure data is chosen with the popup menus in the 'Exposure Data' panel. Select the source data type (dosage, toxic load, internal dose), and discrete thresholds or continuous probit slope dose response curves. Make sure that you have defined the exposure data for the selected source data type in the Toxicity Data Editor, which can be accessed by pressing .

The inhaled internal dose data can be modified by pressing .

The exposure time can be selected at the bottom left-hand corner of the GUI.

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